Variational Constitutive Updates for Strain Gradient Isotropic Plasticity

by

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Abstract

In the past decades, various strain gradient isotropic plasticity theories have been developed to describe the size-dependence plastic deformation mechanisms observed experimentally in micron-indentation, torsion, bending and thin-film bulge tests in metallic materials. Strain gradient plasticity theories also constitute a convenient device to introduce ellipticity in the differential equations governing plastic deformation in the presence of softening. The main challenge to the numerical formulations is that the effective plastic strain, a local internal variable in the classic isotropic plasticity theory, is now governed by the partial differential equation which includes spatial derivatives. Most of the current numerical formulations are based on Aifantis' one-parameter model with a Laplacian term [Aifantis and Muhlhaus, ijss, 28:845-857, 1991]. As indicated in the paper [Fleck and Hutchinson, jmps, 49:2245-2271, 2001], one parameter is not sufficient to match the experimental data. Therefore a robust and efficient computational framework that can deal with more parameters is still in need.

In this thesis, a numerical formulation based on the framework of variational constitutive updates is presented to solve the initial boundary value problem in strain gradient isotropic plasticity. One advantage of this approach compared to the mixed methods is that it avoids the need to solve for both the displacement and the effective plastic strain fields simultaneously. Another advantage of this approach is, as has been amply established for many other material models, that the solution of the problem follows a minimum principle, thus providing a convenient basis for error estimation and adaptive remeshing. The advantages of the framework of variational constitutive updates have already been verified in a wide class of material models including visco-elasticity, visco-plasticity, crystal plasticity and soil, however this approach has not been implemented in the strain gradient plasticity models. In this thesis, a three-parameter strain gradient isotropic plasticity model is formulated within the variational framework, which is then taken as a basis for finite element discretization. The resulting model is implemented in a computer code and exercised on the benchmark problems to demonstrate the robustness and versatility of the proposed method.

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Contents

List of Figures

List of Tables

Chapter 1

Introduction

Plastic deformation on the micron scale plays an important role in a number of technological applications including micro-electronic-mechanical systems (MEMS) and the structural materials, where the components' size as well as the deformation are usually on this scale. Experiments reveal a prominent size-dependence effect for plastic deformation on this scale. Examples of these experiments include the indentation test [28], wire torsion [13], microbend [29] and thin-film bulge [32]. Basically, this size-dependence effect can be stated as *smaller is stronger*. For example, in the wire torsion test [13], the thinner the wire, the stronger the material response. Conventional plasticity theories are unable to explain this effect, because no length scales are considered.

There are different ways to model plastic deformation with size-dependence behavior. The choice of approaches depends on the interest. Dislocation dynamic and molecular dynamic methods are useful to understand the basic physical mechanisms such as the dislocation interactions [33]. Continuum descriptions are needed to describe the effective response and to solve initial boundary value problems, which will be the focus of this thesis.

A number of continuum theories that account for the size-dependence effect in plastic deformation have been proposed. Perhaps owing to their phenomenological nature, there is no consensus on any specific theory. Apparently, the first higher order gradient model can be attributed to Aifantis et al [3]. In order to remove the plastic strain singularity in the presence of softening, they added higher order gradient terms $\nabla^2\epsilon^p$ and $\nabla^4\epsilon^p$ in the conventional flow rule; ϵ^p is the effective plastic strain, and ∇^2 is the usual Laplacian operator. Each new term introduces an internal material length scale as a parameter, which is required by dimensional arguments. These higher order gradient terms bring in the ellipticity to the governing partial differential equations, and consequently eliminate the mesh dependence behavior that appears in the simulation of the plastic flow in the softening regime. Motivated by the size-dependence observed in wire torsion tests, Fleck and Hutchinson formulated a strain gradient plasticity model based on the extensions of the couple stress theory and Toupin-Mindlin theory. In their original model, the gradients of the total strains are considered [11]. Later, they reformulated the model and eliminated the dependence on the gradients of elastic strains because this dependence is not correct in the linear elastic range [12]. Starting from the invariants of the plastic strain gradients $\nabla\mathbf{E}^p$, a third order tensor, they formulated a generalized effective plastic strain which includes three internal material length scales [12]. Based on this generalized effective plastic strain, Fleck and Hutchinson proposed a minimum principle for strain hardening materials, from which the forces balance equations, the boundary conditions and the evolution of the flow stress can be derived straightforwardly through variation. Both Aifantis' model and Fleck and Hutchinson's model (FH mdoel) adopt the conventional normality relation of the isotropic plasticity, i.e. the flow direction is collinear with the deviatoric part of the Cauchy stresses. Regarding the requirement from thermodynamics, some strain gradient plasticity models that do not obey the conventional normality relation are also proposed. Gudmundson generalized the FH model in the sense that the flow direction is collinear with the sum of the deviatoric Cauchy stress tensor and the divergence of the moment stresses (or higher order stresses) which are associated with the plastic strain gradient [16]. Similar to the FH model, three internal material length scales appear in the expression of the generalized effective plastic strain. In parallel to Gudmundson's work, Gurtin and Anand also considered the thermo-dynamic requirement. They proposed a strain gradient plasticity model that involves the back stress and accounts for the visco-plastic effect [17]. The flow stress in their model is assumed to be a power function of the plastic strains and plastic strain gradients. The aforementioned strain gradient plasticity models, with the exception of the visco-plasticity model, have a commonality that the flow stress rate depends linearly on the plastic strain gradient rate. In contrast, Nix and Gao proposed a strain gradient plasticity model (NG model) where the square of the flow stress has a linear dependence on the plastic strain gradient. They based this relation on the analysis of the indentation experiments in [15, 19]. Recently, Evans and Hutchinson assessed the NG model and FH model using the simple bending test as an example [9]. They retained the variational framework of the FH model but modified an exponent in the definition of the generalized effective plastic strain. The resulting model demonstrates that the square of the flow stress depends linearly on the plastic strain gradient as indicated by the NG model, and it also inherits the flexible boundary conditions of the effective plastic strain from the FH model.

Regarding the formulation of numerical methods for strain gradient plasticity models, the main distinction between the gradient and the classic or local models is that the effective plastic strain in the gradient models can not be obtained locally, since its governing partial differential equations include the spatial derivatives. In addition, there is sometimes a need to distinguish the conditions for the boundaries where the dislocations are free to pass by from the boundaries where dislocations are stacked. Examples of the latter case can be found in the passivated layer test in [32]. Popular numerical methods for the classic (or local) models, such as return mapping method, fail to distinguish these two types of boundary conditions, since the measurement of the dislocation density, the effective plastic strain, is not treated as an independent variable.

The initial work on the numerical formulation for strain gradient plasticity should be attributed to de Borst and Muhlhaus [5]. They presented a mixed formulation with the displacement and the effective plastic strain treated as nodal unknowns to simulate the strain softening behavior. In their formulation, Aifantis' one parameter model with Laplacian term is used; the displacement and effective plastic strain fields are updated simultaneously. The same treatment of these two fields was taken in [26, 8] for different strain gradient plasticity models. The main benefit of this simultaneous update is that no additional sensitivity analysis is required, while this treatment has a deficiency that the linear algebraic system to be solved has a huge size. This seems to not be a serious problem for isotropic plasticity, where there are only 4 unknowns per node (3 for the displacement field and 1 for the effective plastic strain field). In the crystal plasticity, however, there are many more unknowns. Take the FCC material as an example. Generally, there are 15 unknowns per node, 3 of which are the displacements and 12 of which are the plastic slips for the 12 slip systems. The linear algebraic system built through the mixed formulation would become too huge to be solvable with current computer systems. Apart from the mixed formulation, some efforts have been made toward developing staggered methods [4, 6, 7]. In these staggered methods, the solution is achieved through a two-level structure. The outer level is the Newton-Raphson iteration for the displacement field and the inner level is the stress update. Once a tentative displacement is obtained from the outer level, the effective plastic strain is solved within the inner level and the stresses are updated consequently. The main advantage of staggered methods is that the algebraic system to be solved is divided into two sub-systems with much smaller sizes, while additional cost of formulating the consistent tangential matrix for the outer level iteration is inevitable. In particular, staggered methods require the sensitivity analysis of the effective plastic strain ϵ^p with respect to the displacement field $\mathbf{u}$, i.e. estimating $\frac{\partial \epsilon^p}{\partial \mathbf{u}}$, which is not trivial due to the nonlocal effect.

In this thesis, a numerical formulation based on the framework of variational constitutive updates is presented to solve the initial boundary value problem in strain gradient isotropic plasticity. The framework of variational constitutive updates was initially laid out by Radovitzky and Ortiz [25] for a wide class of material models, and later applied to a wide variety of specific material phenomena including visco-plasticity [24], viscoelasticity [10], porous elasto-plastic materials [30], soil [23] and nonlinear solid dynamics [22]. The basic idea of variational constitutive updates is that, within each increment in time, the value of internal state variables such as the effective plastic strains can be consistently obtained through the variation of an appropriate functional with respect to appropriate conjugate variables, given the displacement or deformation gradient. Compared to other staggered methods, the solution to the problem will follow from a minimum principle and the symmetry of the consistent tangent matrix is guaranteed. Furthermore, the minimum principle provides a convenient basis for error estimation and adaptive remeshing. The advantages of the framework of variational constitutive updates have already been verified for many material models, however, to the author's knowledge, it has not been implemented on strain gradient plasticity theories. The numerical formulation to be presented employs the FH model [12], which has a relatively simple form and is sufficiently general. In addition, the minimum principle for the incremental version of the FH model provides a solid foundation for variational constitutive updates.

The rest of this thesis is organized as follows. Chapter 2 serves as a brief overview of strain gradient isotropic plasticity models, where only the FH model [12] will be discussed in detail. In Chapter 3, the numerical formulation based on the framework of variational constitutive updates will be presented. In Chapter 4, two numerical examples, shearing of a layer sandwiched by two subtrates and wire torsion, are provided to demonstrate the robustness and efficiency of this numerical formulation. In Chapter 5, the recent improvements on the FH model, the extension of the proposed numerical formulation and the prospects for future work in this area will be discussed.

Chapter 2

Strain gradient models of plasticity

The aforementioned strain gradient plasticity models will be introduced, compared and summarized in this chapter. In particular, the model of Fleck and Hutchinson will be discussed in detail. Notations of the variables that will be frequently used are listed in Table (2.1). Whenever possible, scalars will be indicated by Greek letters, and other variables will be indicated in bold. The rate of a variable $(\bullet)$, i.e. the temporal derivative, is indicated by $(\dot{\bullet})$.

Aifantis' model

In order to eliminate the plastic strain singularity in the presence of softening, Aifantis et al [3, 1] argued that both the effective plastic strain and its gradients must be considered in the expression of flow stress. In these references, he introduced the following constitutive relation

$$\sigma^{fl}(\epsilon^p) = c_0 + c_1 \nabla^2 \epsilon^p + c_2 \nabla^4 \epsilon^p \ , \tag{2.1}$$

where generally $c_i = c_i(\epsilon^p)$. There is an intuitive interpretation of this expression. Assume that

$$\sigma^{fl}(\epsilon^p) = f(\epsilon^p) \tag{2.2}$$

Table 2.1: List of variables

Field	Variable	Components	Comments
displacement	$\mathbf{u}$	u_i	
total strain	$\mathbf{E}$	E_{ij}	$E_{ij} = \frac{1}{2}(u_{i,j} + u_{j,i})$
elastic strain	$\mathbf{E}^e$	E^e_{ij}	
plastic strain	$\mathbf{E}^p$	E^p_{ij}	
effective plastic strain rate	$\dot{\epsilon}^p$		$\dot{\epsilon}^p = \sqrt{\frac{2}{3}\dot{E}^p_{ij}\dot{E}^p_{ij}}$
Cauchy stress	$\mathbf{T}$	T_{ij}	
deviatoric Cauchy stress	$\mathbf{S}$	S_{ij}	$\mathbf{S} = \mathbf{T} - \frac{1}{3}\text{trace}(\mathbf{T})\mathbf{I}$
effective stress	σ^{ef}		$\sigma^{ef} = \sqrt{\frac{3}{2}S_{ij}S_{ij}}$
flow stress	σ^{fl}		

is an expression of the flow stress from the classic (or local) model. The gradients can be naturally included through evaluating f at $\bar{\epsilon^p}$ instead of ϵ^p, i.e.

$$\sigma^{fl}(\epsilon^p) = f(\bar{\epsilon^p}) \ , \tag{2.3}$$

where $\bar{\epsilon^p}$ is an average of ϵ^p in a ball with radius R. If algebraic average is adopted,

$$\bar{\epsilon^p}(\mathbf{x}) = \frac{1}{|B_R|}\int\limits_{B_R} \epsilon^p(\mathbf{x}+\mathbf{r})\, d\mathbf{r} \ . \tag{2.4}$$

Taylor expansion of $\epsilon^p(\mathbf{x}+\mathbf{r})$ at $\mathbf{x}$ yields

$$\epsilon^p(\mathbf{x}+\mathbf{r}) \approx \epsilon^p(\mathbf{x}) + \epsilon^p_{,i}(\mathbf{x})r_i + \frac{1}{2!}\epsilon^p_{,ij}(\mathbf{x})r_ir_j + \frac{1}{3!}\epsilon^p_{,ijk}(\mathbf{x})r_ir_jr_k + \frac{1}{4!}\epsilon^p_{,ijkl}(\mathbf{x})r_ir_jr_kr_l \ .$$

In the volumetric integration of Eq (2.4), terms with odd order derivatives in the Taylor series vanish due to the spheric symmetry. $\bar{\epsilon^p}$ therefore can be approximated by the gradients of ϵ^p as

$$\bar{\epsilon^p}(\mathbf{x}) \approx \epsilon^p(\mathbf{x}) + \frac{1}{|B_R|}\left(\frac{1}{2!}\frac{4\pi R^5}{15}\nabla^2\epsilon^p(\mathbf{x}) + \frac{1}{4!}\frac{4\pi R^7}{35}\nabla^4\epsilon^p(\mathbf{x})\right) . \tag{2.5}$$

Linearization of $f(\bar{\epsilon^p})$ at ϵ^p leads to

$$f(\bar{\epsilon^p}) \approx f(\epsilon^p) + h(\epsilon^p)(\bar{\epsilon^p} - \epsilon^p) \tag{2.6}$$

where $h(\epsilon^p) = f'(\epsilon^p)$ is identified as hardening function. With these preparations, the flow stress can be reformulated as follows.

$$\begin{aligned}
\sigma^{fl}(\epsilon^p) &= f(\bar{\epsilon^p}) \\
&\approx f(\epsilon^p) + h(\epsilon^p)(\bar{\epsilon^p} - \epsilon^p) \\
&= f(\epsilon^p) + h(\epsilon^p)\frac{1}{|B_R|}\left(\frac{1}{2!}\frac{4\pi R^5}{15}\nabla^2\epsilon^p + \frac{1}{4!}\frac{4\pi R^7}{35}\nabla^4\epsilon^p\right) \\
&= f(\epsilon^p) + h(\epsilon^p)\left(\frac{R^2}{10}\nabla^2\epsilon^p + \frac{R^4}{280}\nabla^4\epsilon^p\right) .
\end{aligned}$$

This suggests

$$c_0 = f(\epsilon^p)\ , \quad c_1 = h(\epsilon^p)\tfrac{R^2}{10}\ , \quad c_2 = h(\epsilon^p)\tfrac{R^4}{280}$$

in the expression of flow stress (Eq (2.1))

$$\sigma^{fl}(\epsilon^p) = c_0 + c_1\nabla^2\epsilon^p + c_2\nabla^4\epsilon^p\ .$$

And radius R can be viewed as a problem specific internal length scale.

The foregoing interpretation has a limitation that c_1 and c_2 are forced to take the same sign. The ellipticity is then only valid if h does not change sign during the entire deformation. $h > 0$ represents hardening and $h < 0$ represents softening. In some situation, it is desirable to include both hardening and softening behaviors in the deformation. Based on this consideration, Aifantis argued that the interpretation above is not necessary, and the coefficients c_1 and c_2 can be independent of each other.

Later, Aifantis also utilized his proposed gradient model to describe the size-dependence effects [2]. The expressions of the flow stress he presented later are more general than Eq (2.1). Other gradient terms such as $\|\nabla\epsilon^p\|_2$ also appear in the constitutive relation in order to fit the experimental results. Among all of the strain gradient plasticity models proposed by Aifantis, the model described by the equation

$$\sigma^{fl}(\epsilon^p) = \sigma^0 + h\epsilon^p + c\nabla^2\epsilon^p \ . \tag{2.7}$$

is the simplest and most popular in the formulation of numerical methods.

Fleck and Hutchinson's model

The frame of variational constitutive updates to be presented in the next chapter is inspired by the strain gradient plasticity model of Fleck and Hutchinson [12]. Starting from the invariants of the plastic strain gradients $\nabla\mathbf{E}^p$, Fleck and Hutchinson constructed a generalized effective plastic strain rate, and then proposed a minimum principle for strain hardening materials. This minimum principle is an extension of the extremum principle by Hill for the classical case of isotropic hardening materials. Unlike Aifantis' models where the expression of flow stress is imposed a priori, the flow rule is naturally generated from the optimal conditions of the proposed minimum principle.

Basic assumptions in small strain isotropic plasticity are adopted, such as the additive decomposition of elastic and plastic strains, small rotation and incompressibility of plastic deformation. These assumptions can be mathematically expressed as

$$\mathbf{E} = \mathbf{E}^e + \mathbf{E}^p \ , \quad \text{trace}(\mathbf{E}^p) = 0 \ .$$

The normality condition

$$\dot{\mathbf{E}}^p = \begin{cases} \dot{\epsilon}^p\mathbf{N} = \dot{\epsilon}^p\frac{3}{2}\frac{\mathbf{S}}{\sigma^{ef}} & \text{upon plastic loading} \\ 0 & \text{otherwise} \end{cases}$$

from J_2 flow theory is also adopted, leaving the definition of plastic loading to be determined.

It is an important feature of the FH model that higher order stresses associated with plastic strain gradients are explicitly introduced in the model, and the Principle of Virtual Work is utilized to obtain the equilibrium equations. The Principle of Virtual Work in the FH model can be expressed in the following way.

$$
\begin{aligned}
& \text{Internal virtual work:} \\
= \;& \textstyle\int_V T_{ij}\delta E^e_{ij} + \Sigma\delta\epsilon^p + m_i\delta\epsilon^p_{,i}\, dV \\
= \;& \textstyle\int_V T_{ij}(\delta E_{ij} - \delta E^p_{ij}) + \Sigma\delta\epsilon^p + m_i\delta\epsilon^p_{,i}\, dV \\
= \;& \textstyle\int_V T_{ij}\delta E_{ij} - S_{ij}\delta E^p_{ij} + \Sigma\delta\epsilon^p + m_i\delta\epsilon^p_{,i}\, dV \\
= \;& \textstyle\int_V T_{ij}\delta E_{ij} - S_{ij}\delta\epsilon^p N_{ij} + \Sigma\delta\epsilon^p + m_i\delta\epsilon^p_{,i}\, dV \\
= \;& \textstyle\int_V T_{ij}\delta E_{ij} - \sigma^{ef}\delta\epsilon^p + \Sigma\delta\epsilon^p + m_i\delta\epsilon^p_{,i}\, dV \\
= \;& \textstyle\int_V -T_{ij,j}\delta u_i + (\Sigma - \sigma^{ef} - m_{i,i})\delta\epsilon^p\, dV + \int_S T_{ij}n_j\delta u_i + m_i n_i\delta\epsilon^p\, dS \\
= \;& \text{External virtual work} \\
= \;& \textstyle\int_S t_i\delta u_i + \tau\delta\epsilon^p\, dS
\end{aligned}
\tag{2.8}
$$

where Σ and $\mathbf{m}$ are the work-conjugates to the effective plastic strain and plastic strain gradients respectively, $\mathbf{t}$ and τ are the traction and higher order traction prescribed on the boundary respectively, and $\mathbf{n}$ is the outer normal direction to the boundary. Regarding the dimension, $\mathbf{m}$ is called the higher order stresses (or moment stresses). The local equilibrium equations follow immediately from the variational equation (2.8).

In the body, we have

$$T_{ij,j} = 0 \tag{2.9}$$

$$\Sigma - \sigma^{ef} - m_{i,i} = 0\,. \tag{2.10}$$

While on the boundary, we get

$$t_i = T_{ij}n_j \tag{2.11}$$

$$\tau = m_i n_i\,. \tag{2.12}$$

In addition to the conventional equilibrium equations Eq (2.9, 2.11), Eq (2.10) and Eq (2.12) emerge resulting from the variation with respect to ϵ^p. In the Principle of

Virtual Work (Eq (2.8)), Σ is the work-conjugate to the effective plastic strain, while in the classical J_2 flow theory, it is the effective stress σ^{ef} that serves as the work-conjugate to the effective plastic strain. Σ is therefore called the generalized effective stress. Fleck and Hutchinson specified the plastic loading in the their gradient model by

$$\Sigma = \Sigma^Y \quad \text{and} \quad \dot{\Sigma} = \dot{\Sigma}^Y \tag{2.13}$$

where Σ^Y is called generalized yield stress. The gradient model of Fleck and Hutchinson will be complete if the evolution of Σ^Y is described.

Inspired by the minimum principle of Hill for strain hardening materials in the classic J_2 flow theory, Fleck and Hutchinson proposed the following minimum principle[1]: among all the kinematically admissible fields, the exact rates of the displacement and the effective plastic strain minimizes the following functional

$$I(\dot{\mathbf{u}}, \dot{\epsilon}^p) = \frac{1}{2}\int_V C_{ijkl}(\dot{E}_{ij} - \dot{\epsilon}^p N_{ij})(\dot{E}_{kl} - \dot{\epsilon}^p N_{kl}) + h(\Lambda^p)(\dot{\Lambda}^p)^2 \, dV - \int_{S_T} \dot{t}_i \dot{u}_i + \dot{\tau}\dot{\epsilon}^p \, dS \, . \tag{2.14}$$

In Eq (2.14), $\mathbf{C}$ is the conventional fourth order elasticity tensor, the hardening function h that comes from uniaxial tensile test is always positive and $\dot{\Lambda}^p$ is the generalized effective plastic strain rate defined by the expression

$$\dot{\Lambda}^p = \left\{(\dot{\epsilon}^p)^2 + A_{ij}\dot{\epsilon}^p_{,i}\dot{\epsilon}^p_{,j} + B_i\dot{\epsilon}^p_{,i}\dot{\epsilon}^p + C(\dot{\epsilon}^p)^2\right\}^{\frac{1}{2}} \, . \tag{2.15}$$

The coefficients A_{ij}, B_i and C are dependent on internal material length scales. Expressions of these coefficients are given in Appendix A.9.

It is shown in Appendix (A.22, A.27) that the minimum $\{\dot{\mathbf{u}}, \dot{\epsilon}^p\}$ of I should satisfy

[1] Proof of this minimum principle is provided in Appendix (Theorem 1).

the following optimality conditions:

$$\begin{aligned} \dot{T}_{ij,j} &= 0 \quad \text{in } V \\ \dot{T}_{ij}n_j &= \dot{t}_i \quad \text{on } S_T \\ -\dot{\sigma}^{ef} + h[(1+C)\dot{\epsilon}^p + \tfrac{1}{2}B_i\dot{\epsilon}^p_{,i}] - \{h[A_{ij}\dot{\epsilon}^p_{,j} + \tfrac{1}{2}B_i\dot{\epsilon}^p]\}_{,i} &= 0 \quad \text{in } V \\ h[A_{ij}\dot{\epsilon}^p_{,j} + \tfrac{1}{2}B_i\dot{\epsilon}^p]n_i &= \dot{\tau} \quad \text{on } S_T \end{aligned} \tag{2.16}$$

where $\dot{\mathbf{T}}$ is the rate of Cauchy stresses associated with $\{\dot{\mathbf{u}}, \dot{\epsilon}^p\}$.

In consistency with the conclusions derived from the Principle of Virtual Work (Eq (2.10, 2.12)), it is natural to define

$$\dot{m}_i = h[A_{ij}\dot{\epsilon}^p_{,j} + \frac{1}{2}B_i\dot{\epsilon}^p] \ , \tag{2.17}$$

and

$$\dot{\Sigma}^Y = h[(1+C)\dot{\epsilon}^p + \frac{1}{2}B_i\dot{\epsilon}^p_{,i}] \ . \tag{2.18}$$

After applying these definitions, variational results in Eq (2.16) become identical to the rate form of the PVW results (Eq (2.9, 2.10, 2.11, 2.12)) upon plastic loading. Equations that govern the evolution of this elastic-plastic body are summarized below.

Equilibrium equations:

$$T_{ij,j} = 0 \tag{2.19}$$

$$\Sigma - \sigma^{ef} - m_{i,i} = 0 \tag{2.20}$$

$$T_{ij}n_j = t_i \quad \text{on } S_T \times (0, T^f] \tag{2.21}$$

$$m_i n_i = \tau \quad \text{on } S_T \times (0, T^f] \tag{2.22}$$

Constitutive equations:

$$T_{ij} = C_{ijkl}E^e_{ij} \tag{2.23}$$

$$\dot{E}^p_{ij} = \dot{\epsilon}^p N_{ij} \tag{2.24}$$

$$N_{ij} = \frac{3}{2\sigma^{ef}}S_{ij} \tag{2.25}$$

$$S_{ij} = T_{ij} - \frac{1}{3}T_{kk} \tag{2.26}$$

$$\dot{\epsilon}^p(\Sigma - \Sigma^Y) = 0 \tag{2.27}$$

$$\dot{\epsilon}^p \geq 0 \tag{2.28}$$

$$\Sigma - \Sigma^Y \leq 0 \tag{2.29}$$

$$\dot{m}_i = h(\Lambda^p)[A_{ij}\dot{\epsilon}^p_{,j} + \frac{1}{2}B_i\dot{\epsilon}^p] \tag{2.30}$$

$$\dot{\Sigma}^Y = h(\Lambda^p)[(1+C)\dot{\epsilon}^p + \frac{1}{2}B_i\dot{\epsilon}^p_{,i}] \tag{2.31}$$

$$\dot{\Lambda}^p = \left\{(\dot{\epsilon}^p)^2 + A_{ij}\dot{\epsilon}^p_{,i}\dot{\epsilon}^p_{,j} + B_i\dot{\epsilon}^p_{,i}\dot{\epsilon}^p + C(\dot{\epsilon}^p)^2\right\}^{\frac{1}{2}} \tag{2.32}$$

Compatibility equations:

$$E_{ij} = \frac{1}{2}(u_{i,j} + u_{j,i}) \tag{2.33}$$

$$E_{ij} = E^e_{ij} + E^p_{ij} \tag{2.34}$$

$$\sigma^{ef} = \sqrt{\frac{3}{2}S_{ij}S_{ij}} \tag{2.35}$$

$$u_i = u^S_i \quad \text{on } S_U \times (0, T^f] \tag{2.36}$$

$$\epsilon^p = \epsilon^{p,S} \quad \text{on } S_U \times (0, T^f] \tag{2.37}$$

Initial conditions:

$$u_i = u^0_i \quad \text{on } \bar{V} \times \{0\} \tag{2.38}$$

$$\epsilon^p = \epsilon^{p,0} \quad \text{on } \bar{V} \times \{0\} \tag{2.39}$$

$$\Lambda^p = \left\{(\epsilon^{p,0})^2 + A_{ij}\epsilon^{p,0}_{,i}\epsilon^{p,0}_{,j} + B_i\epsilon^{p,0}_{,i}\epsilon^{p,0} + C(\epsilon^{p,0})^2\right\}^{\frac{1}{2}} \quad \text{on } \bar{V} \times \{0\} \tag{2.40}$$

In the collection of equations above, h, u^S_i, $\epsilon^{p,S}$, u^0_i and $\epsilon^{p,0}$ are known functions and $[0, T^f]$ is the total time interval of the evolution.

Gudmundson's model

Gudmundson generalized the Principle of Virtual Work that has been used by Fleck and Hutchinson, where the full plastic strain tensor instead of the effective plastic strain is considered [16]. Another important feature of Gudmundson's model is that the classic assumption of normality of the plastic flow is abandoned.

The principle of virtual work in Gudmundson's model reads

$$
\begin{aligned}
& \text{Internal virtual work:} \\
= \;& \int_V T_{ij}\delta E^e_{ij} + Q_{ij}\delta E^p_{ij} + M_{ijk}\delta E^p_{ij,k}\, dV \\
= \;& \int_V T_{ij}(\delta E_{ij} - \delta E^p_{ij}) + Q_{ij}\delta E^p_{ij} + M_{ijk}\delta E^p_{ij,k}\, dV \\
= \;& \int_V T_{ij}\delta E_{ij} + (Q_{ij} - S_{ij})\delta E^p_{ij} + M_{ijk}\delta E^p_{ij,k}\, dV \\
= \;& \int_V -T_{ij,j}\delta u_i + (Q_{ij} - S_{ij} - M_{ijk,k})\delta E^p_{ij}\, dV + \int_S T_{ij}n_j\delta u_i + M_{ijk}n_k\delta E^p_{ij}\, dS \\
= \;& \text{External virtual work} \\
= \;& \int_S t_i\delta u_i + R_{ij}\delta E^p_{ij}\, dS\ ,
\end{aligned}
\tag{2.41}
$$

where $\mathbf{Q}$ and $\mathbf{M}$ are the work-conjugates to the plastic strain $\mathbf{E}^p$ and its gradient respectively, $\mathbf{t}$ and $\mathbf{R}$ are the traction and the higher order traction prescribed at the boundary respectively, and $\mathbf{n}$ is the outward normal to the boundary. The local equilibrium equations follow directly from the variational equation (2.41).

$$
\begin{aligned}
T_{ij,j} &= 0 \quad \text{in } V\ , \\
Q_{ij} - S_{ij} - M_{ijk,k} &= 0 \quad \text{in } V\ , \\
T_{ij}n_j &= t_i \quad \text{on } S\ , \\
M_{ijk}n_k &= R_{ij} \quad \text{on } S\ .
\end{aligned}
\tag{2.42}
$$

Rather than simply accepting the normality relation in classic J_2 flow theory, Gudmundson brought in the free energy and derived the normality relation based on the plastic dissipation. Assume that the free energy density is $\psi(E^e_{ij}, E^p_{ij}, E^p_{ij,k})$. The plastic dissipation has the following formula

$$
\begin{aligned}
\mathscr{D} &= \int_{V_e} (T_{ij} - \frac{\partial \psi}{\partial E^e_{ij}})\dot{E}^e_{ij} + (Q_{ij} - \frac{\partial \psi}{\partial E^p_{ij}})\dot{E}^p_{ij} + (M_{ijk} - \frac{\partial \psi}{\partial E^p_{ij,k}})\dot{E}^p_{ij,k}\, dV \\
&= \int_{V_e} (Q_{ij} - \frac{\partial \psi}{\partial E^p_{ij}})\dot{E}^p_{ij} + (M_{ijk} - \frac{\partial \psi}{\partial E^p_{ij,k}})\dot{E}^p_{ij,k}\, dV \ ,
\end{aligned}
\tag{2.43}
$$

where V_e is an arbitrary volume element. This expression can be simplified as

$$
\mathscr{D} = \int_{V_e} \bar{Q}_{ij}\dot{E}^p_{ij} + \bar{M}_{ijk}\dot{E}^p_{ij,k}\, dV \ . \tag{2.44}
$$

if definitions $\bar{Q}_{ij} = Q_{ij} - \frac{\partial \psi}{\partial E^p_{ij}}$ and $\bar{M}_{ijk} = M_{ijk} - \frac{\partial \psi}{\partial E^p_{ij,k}}$ are applied.

As an analogue to the principle of maximum plastic work in the classic J_2 theory, if the plastic strain and strain gradients are prescribed, the actual stresses pair $\{\bar{Q}_{ij}, \bar{M}_{ijk}\}$ will maximize the plastic work, i.e.

$$
\{\bar{Q}_{ij}, \bar{M}_{ijk}\} = arg \max_{\{\bar{Q}^*_{ij}, \bar{M}^*_{ijk}\} \in \mathbb{E}} \bar{Q}^*_{ij}\dot{E}^p_{ij} + \bar{M}^*_{ijk}\dot{E}^p_{ij,k} \tag{2.45}
$$

where $\mathbb{E}$ is the current yield surface with the definition[2]

$$
\mathbb{E} = \left\{ \{\bar{Q}^*_{ij}, \bar{M}^*_{ijk}\} | \sqrt{\frac{3}{2}\bar{Q}^*_{ij}\bar{Q}^*_{ij} + L^{-2}\bar{M}^*_{ijk}\bar{M}^*_{ijk}} \leq \Sigma^Y \right\} \ .
$$

In the definition above, L is the characteristic material length scale and Σ^Y is the generalized yield stress.

The Lagrange function associated with the constrained optimization problem (2.45) is

$$
\mathscr{L}(\bar{Q}^*_{ij}, \bar{M}^*_{ijk}, \lambda^*) = \bar{Q}^*_{ij}\dot{E}^p_{ij} + \bar{M}^*_{ijk}\dot{E}^p_{ij,k} + \lambda^* \left(\sqrt{\frac{3}{2}\bar{Q}^*_{ij}\bar{Q}^*_{ij} + L^{-2}\bar{M}^*_{ijk}\bar{M}^*_{ijk}} - \Sigma^Y \right) \ , \tag{2.46}
$$

[2]This definition is a simplified version of the one in Gudmundson's paper. He also utilized the orthogonal decomposition of the third order tensors so that three characteristic material length scales are included. Nevertheless, this simplified version already contains the essential structure.

where λ is a multiplier corresponding to the inequality constraint. Assume $(\mathbf{Q}, \mathbf{M})$ is the maximum and λ is the associated multiplier. First order necessary conditions for the constrained optimization problem (2.45) then read

$$\frac{\partial \mathscr{L}}{\partial \bar{Q}^*_{ij}}(\mathbf{Q}, \mathbf{M}, \lambda) = 0 \quad \text{and} \quad \frac{\partial \mathscr{L}}{\partial \bar{M}^*_{ijk}}(\mathbf{Q}, \mathbf{M}, \lambda) = 0 \ ,$$

which yield the following normality relations

$$\begin{cases} \dot{E}^p_{ij} &= \lambda \frac{3}{2}\frac{1}{\Sigma}\bar{Q}_{ij} \\ \dot{E}^p_{ij,k} &= \lambda \frac{1}{\Sigma} L^{-2} \bar{M}_{ijk} \end{cases} \tag{2.47}$$

with definitions

$$\begin{cases} \Sigma = \sqrt{\frac{3}{2}\bar{Q}_{ij}\bar{Q}_{ij} + L^{-2}\bar{M}_{ijk}\bar{M}_{ijk}} \\ \lambda = \sqrt{\frac{2}{3}\dot{E}^p_{ij}\dot{E}^p_{ij} + L^2 \dot{E}^p_{ij,k}\dot{E}^p_{ij,k}} \end{cases} .$$

In order to complete Gudmundson's model, an expression for the free energy density ψ must be provided. A sample expression

$$\psi(E^e_{ij}, E^p_{ij}, E^p_{ij,k}) = \frac{1}{2} C_{ijkl} E^e_{ij} E^e_{kl} + \mu L^2 E^p_{ij,k} E^p_{ij,k}$$

is offered in his paper where μ is the shear modulus. $\dot{E}^p_{ij}$ is usually not included in the free energy density expression, so the first equation in (2.47) can be rewritten as

$$\dot{E}^p_{ij} = \lambda \frac{3}{2}\frac{1}{\Sigma} Q_{ij} \ .$$

Gurtin and Anand's model

Not long after Gudmundson's work, Gurtin and Anand proposed a strain gradient visco-plasticity model [17]. They also abandoned the classical assumption of normality of the flow rule regarding the non-negative requirement of plastic dissipation. When they apply the Principle of Virtual Work, the full plastic strain tensor is used, so the equilibrium equations they obtained coincide with those in Eq (2.42). An important feature of Gurtin and Anand's model is that the expression of the free energy density is specified, where only the curl of the plastic strain gradient (curl$\mathbf{E}^p$) rather than the full tensor ($\nabla\mathbf{E}^p$) is included. They made this choice because the curl of the plastic strain tensor is a measure of the incompatibility of the plastic strain field and in the micro-structural configuration, it measures the local Burgers vector [18] while other components of the plastic strain gradient tensor do not have such physical meanings. In their formulation, they also distinguished the characteristic material length scales in the expression of the free energy density and those in the expression of the generalized effective plastic strain rate. The length scales in the expression of the free energy density are identified as the energetic length scales because these length scales only appear in the back stress term in the flow rule (2.50), which represents the energy stored in the material due to the incompatibility of the deformation. The length scales in the expression of the generalized effective plastic strain rate are identified as the dissipative length scales, because they only appear in the dissipative terms in the flow rule, which presents the energy dissipated during the plastic deformation. A sample expression of free energy density in their paper reads

$$\psi = \frac{1}{2}C_{ijkl}E^e_{ij}E^e_{kl} + \frac{1}{2}\mu L^2 \varepsilon_{ist}E^p_{jt,s}\varepsilon_{imn}E^p_{jn,m} \,. \tag{2.48}$$

In Gudmundson's model, the normality relations (2.47) are derived from the first order necessary conditions associated with the constrained optimization problem (2.45). As a result, the two equations in (2.47) have a common Lagrange multiplier. In Gurtin and Anand's work, they did not take the principle of maximum plastic work as a point of departure. Instead, they proposed the following normality relations that account for the visco-plasticity effects:

$$\begin{cases} Q_{ij} &= S(\frac{d^p}{d_0})^m \frac{1}{d^p}\dot{E}^p_{ij} \\ \bar{M}_{ijk} &= l^2 S^Y(\frac{d^p}{d_0})^m \frac{1}{d^p}\dot{E}^p_{ij,k} \,, \end{cases} \tag{2.49}$$

where

$$d^p = \sqrt{\dot{E}^p_{ij}\dot{E}^p_{ij} + l^2\dot{E}^p_{ij,k}\dot{E}^p_{ij,k}} \,,$$

and S is an internal variable whose evolution is characterized by

$$\dot{S} = H(S)d^p, \quad S(x,0) = S^Y .$$

It is worth emphasizing that the non-negativeness of the plastic work in Gurtin and Anand's model is guaranteed since the normality equations (2.49) implies that the plastic work

$$Q_{ij}\dot{E}^p_{ij} + \bar{M}_{ijk}\dot{E}^p_{ij,k} = (\frac{d^p}{d_0})^m \frac{1}{d^p}\dot{E}^p_{ij}\dot{E}^p_{ij} + l^2 S^Y (\frac{d^p}{d_0})^m \frac{1}{d^p}\dot{E}^p_{ij,k}\dot{E}^p_{ij,k} \geq 0 .$$

Combination of Eq (2.49) and the second equation of (2.42) yields

$$\begin{aligned} S_{ij} - &\underbrace{(-1)\mu L^2[E^p_{ij,pp} - \frac{1}{2}(E^p_{ik,jk} + E^p_{jk,ik}) + \frac{1}{3}(\delta_{ij}E^p_{rk,rk})]}_{\text{energetic backstress}} \\ &= \underbrace{S(\frac{d^p}{d_0})^m \frac{\dot{E}^p_{ij}}{d^p} - l^2 S_Y[(\frac{d^p}{d_0})^m \frac{\dot{E}^p_{ij,k}}{d^p}]_{,k}}_{\text{dissipative hardening}} , \end{aligned} \tag{2.50}$$

which is the flow rule of Gurtin and Anand's model.

Nix and Gao's model

Motivated by their analysis of indentation experiments, Nix and Gao proposed a mechanism-based theory of strain gradient plasticity [15, 19]. The main result is that the square of the flow stress is an affine function of the plastic strain gradient, i.e.

$$\sigma^{fl} = \sigma^Y_0 \sqrt{f^2(\epsilon) + l\eta} \tag{2.51}$$

where σ^Y_0 is the initial yield stress, f is a function characterizing the uniaxial stress-strain curve in the absence of the gradient effect, $\epsilon = \sqrt{\frac{2}{3}E_{ij}E_{ij}}$ is the effective strain, η is the effective strain gradient, and l is an internal material length scale.

Expression (2.51) is derived from the Taylor relation of the shear strength and the dislocation density. The Taylor relation predicts that

$$\tau = \alpha\mu b\sqrt{\rho_T}\ , \tag{2.52}$$

where τ is the shear strength, μ is the shear modulus, b is the magnitude of the Burgers vector, ρ_T is the total dislocation density, and α is an empirical constant. Assume that von Mises criterion is adopted and the total dislocation density is simply the sum of the statistically stored dislocation density ρ_S and the geometrically necessary dislocation density ρ_G. Eq (2.52) can therefore be reformulated as

$$\sigma^{fl} = \sqrt{3}\tau = \sqrt{3}\alpha\mu b\sqrt{\rho_S + \rho_G}\ . \tag{2.53}$$

In the absence of gradient effects, ρ_G vanishes and then

$$\sigma^{fl} = \sqrt{3}\alpha\mu b\sqrt{\rho_S} = \sigma_0^Y f(\epsilon)\ ,$$

which implies

$$\sqrt{3}\alpha\mu b\sqrt{\rho_S} = \sigma_0^Y f(\epsilon)\ . \tag{2.54}$$

Nix and Gao defined the effective strain gradient as

$$\eta = \rho_G b\ , \tag{2.55}$$

considering the dimensional requirement and some geometrical insight. Effective strain gradient η defined in Eq (2.55) can be viewed as the curvature of the bending [13] and the twist per unit length in the wire torsion tests [15].

Combination of Eq (2.53, 2.54, 2.55) yields the expression of flow stress in Eq (2.51) with the value of the internal material length scale $l = 3\alpha^2(\frac{\mu}{\sigma_0^Y})^2 b$.

Chapter 3

Numerical methods for strain gradient isotropic plasticity

3.1 Summary of current numerical methods

The initial work on the formulation of numerical methods for strain gradient plasticity should be attributed to de Borst and Mühlhaus [5]. In their paper, they used Aifantis' one parameter model (2.7) to provide the ellipticity of the governing partial differential equations in the strain-softening regime. The numerical formulation proposed by de Borst and Mühlhaus is a mixed method in the sense that the displacement and the effective plastic strain are treated as nodal unknowns and updated simultaneously. Another important feature of their approach is that weak formulation has been applied on both the conventional equilibrium equation and the yield condition, so that the yield condition is satisfied in the sense of distributions rather than point-wise. de Borst and Mühlhaus did not take the Principle of Virtual Work as a point of departure; consequently the concept of higher order stresses does not emerge in the formulation. Only the conventional traction condition is applied on the boundary. A potential theoretical issue with this approach is that, resulting from the weak formulation, either the value of $\dot{\epsilon}^p$ or $\dot{\epsilon}^p_{,i} n_i$ should be prescribed at the elastic–plastic boundary. Regarding the continuity of the plastic strain field, they imposed $\dot{\epsilon}^p = 0$ at the internal elastic–plastic boundary. A numerical example of a bar with imperfections at the center under uniaxial tension is used to demonstrate that the mesh-dependence effect is eliminated during the plastic deformation with softening.

Following the approach of de Borst and Mühlhaus, Ramaswamy and Aravas [26] applied the mixed formulation to a two-dimensional problem, localization of plastic flow in plane strain tension. A general expression of flow stress

$$\sigma^{ef} = \sigma^0 \left(g(\epsilon^p) + l_1\, g_1(\epsilon^p) \|\nabla \epsilon^p\|_2 + l_2^2\, g_2(\epsilon^p) \nabla^2 \epsilon^p \right)$$

is adopted in the formulation they proposed, although in the numerical example, the degenerate case with $l_1 = 0$ and $g_2 \equiv -1$ is used, which is almost the same as Aifantis' one parameter model (2.7). Engelen, Geers and Baaijens also took the approach of mixed formulations to simulate plastic deformation in the presence of strain-softening [8]. They introduced a so-called implicit gradient model

$$\bar{\epsilon}^p - c(l)\nabla^2 \bar{\epsilon}^p = \epsilon^p \ , \tag{3.1}$$

where $\bar{\epsilon}^p$ is a nonlocal measure of the plastic strain. Instead of ϵ^p, $\bar{\epsilon}^p$ is considered as the primary unknown. The main advantage of this implicit model is that no additional condition is needed on the internal elastic-plastic boundary, since Eq (3.1) is assumed valid throughout the domain. On the external boundary, $\bar{\epsilon}^p_{,i} n_i = 0$ is set to ensure that same amount of plastic deformation will be obtained no matter whether ϵ^p or $\bar{\epsilon}^p$ is chosen to measure the plastic deformation, i.e.

$$\int_V \bar{\epsilon}^p \, dV = \int_V \epsilon^p \, dV \ .$$

In addition to the mixed formulations, efforts have been made to develop the methods where the displacement and the effective plastic strain are not updated simultaneously [21, 4, 6, 7]. In [21] and [4], the effective plastic strain ϵ^p is defined at Gaussian points instead of nodes. Each Gaussian point is assigned a 'super-element', which comprises several adjacent elements in its neighborhood. ϵ^p is then approximated by a quadratic polynomial using the least square method within this super-element. The increment of ϵ^p at each Gaussian point is directly obtained from the solution of the linearized yield condition within the corresponding super-element, given the strain increment. The main appeal of this approach is that the displacement is the only nodal unknown, which makes it possible to utilize the existing finite element code without significant modification in structure. Nevertheless, this approach means that the solution to a globally existing second order partial differential equation including spatial derivatives is obtained within patches (super-element). It is not clear how to assign boundary conditions for these patches, and a more serious issue is that the accuracy of such approximations is not guaranteed theoretically. Recently, Djoko, Ebobisse, McBride and Reddy implemented a staggered method in the framework of discontinuous Galerkin formulations for plane problems [6, 7]. The effective plastic strain is discretized by discontinuous piecewise-linear elements. Aifantis's one parameter model is utilized in their formulation to demonstrate the size-dependence effects.

3.2 Variational constitutive updates applied to Fleck and Hutchinson's model

As already mentioned in Chapter 1, the numerical formulation based on the framework of variational constitutive updates provides an alternative approach for solving the initial boundary value problem for strain gradient plasticity theories. The key element of building a numerical formulation that adopts this framework is to construct an appropriate functional, from which the internal variables can be obtained through minimization. Due to its minimum structure, the incremental version of the strain gradient isotropic model proposed by Fleck and Hutchinson is taken as the foundation of the numerical formulation in this thesis.

Assume that the displacement rate $\dot{\mathbf{u}}$ is tentatively prescribed, which implies that the strain rate $\dot{\mathbf{E}}$ is also determined. The effective plastic strain rate $\dot{\epsilon}^p$ can be consistently obtained through the variation of the functional in (2.14) with respect to the effective plastic strain, i.e.

$$\dot{\epsilon}^p = arg \min_{\tilde{\epsilon}^p} J(\tilde{\epsilon}^p; \dot{\mathbf{u}}) \ . \tag{3.2}$$

with

$$J(\dot{\epsilon}^p; \dot{\mathbf{u}}) = \frac{1}{2} \int_V C_{ijkl}(\dot{E}_{ij} - \dot{\epsilon}^p N_{ij})(\dot{E}_{kl} - \dot{\epsilon}^p N_{kl}) + h(\Lambda^p)(\dot{\Lambda}^p)^2 \, dV - \int_{S_T} \dot{\tau}\dot{\epsilon}^p + \dot{t}_i \dot{u}_i \, dS \ .$$

Consistency is satisfied in the sense that if the strain rate is the exact rate, the effective plastic strain rate obtained from the variational constitutive update will satisfy the force balance equations and the constitutive equations in (2.16). The stress update follows immediately from the solution to the minimization problem (3.2)

$$\dot{T}_{ij} = C_{ijkl}(\dot{E}_{kl} - \dot{\epsilon}^p N_{kl}) \ .$$

Considering the definition of the generalized effective plastic strain rate (2.15)

$$(\dot{\Lambda}^p)^2 = (\dot{\epsilon}^p)^2 + A_{ij}\dot{\epsilon}^p_{,i}\dot{\epsilon}^p_{,j} + B_i \dot{\epsilon}^p_{,i}\dot{\epsilon}^p + C(\dot{\epsilon}^p)^2 \ ,$$

the expression of the functional in (3.2) can be reformulated as follows.

$$\begin{aligned} J(\dot{\epsilon}^p; \dot{\mathbf{u}}) &= \frac{1}{2} \int_V C_{ijkl}(\dot{E}_{ij} - \dot{\epsilon}^p N_{ij})(\dot{E}_{kl} - \dot{\epsilon}^p N_{kl}) + h(\Lambda^p)(\dot{\Lambda}^p)^2 \, dV - \int_{S_T} \dot{\tau}\dot{\epsilon}^p + \dot{t}_i \dot{u}_i \, dS \\ &= \frac{1}{2} \int_V M_{ij} e_i e_j - 4\mu N_{ij} \dot{E}_{ij} \dot{\epsilon}^p + C_{ijkl}\dot{E}_{ij}\dot{E}_{kl} \, dV - \int_{S_T} \dot{\tau}\dot{\epsilon}^p + \dot{t}_i \dot{u}_i \, dS \\ &= \frac{1}{2} \int_V M_{ij} e_i e_j \, dV - \int_V 2\mu N_{ij} \dot{E}_{ij} \dot{\epsilon}^p \, dV - \int_{S_T} \dot{\tau}\dot{\epsilon}^p \, dS \\ &\quad + \frac{1}{2} \int_V C_{ijkl}\dot{E}_{ij}\dot{E}_{kl} \, dV - \int_{S_T} \dot{t}_i \dot{u}_i \, dS \end{aligned} \tag{3.3}$$

with

$$\mathbf{e} = \left[\dot{\epsilon}^p_{,1}, \ \dot{\epsilon}^p_{,2}, \ \dot{\epsilon}^p_{,3}, \ \dot{\epsilon}^p\right]^T \tag{3.4}$$

and

$$\mathbf{M} = \begin{bmatrix} hA_{11} & hA_{12} & hA_{13} & h\frac{1}{2}B_1 \\ hA_{21} & hA_{22} & hA_{23} & h\frac{1}{2}B_2 \\ hA_{31} & hA_{32} & hA_{33} & h\frac{1}{2}B_3 \\ h\frac{1}{2}B_1 & h\frac{1}{2}B_2 & h\frac{1}{2}B_3 & h(1+C)+3\mu \end{bmatrix} . \tag{3.5}$$

$\mathbf{M}$ is positive definite and symmetric due to the definition of $\dot{\Lambda}^p$[1]. Provided that $\mathbf{N}$ does not degenerate to zero,

$$\begin{aligned} C_{ijkl}N_{kl}N_{ij} &= \lambda\delta_{ij}\delta_{kl} + \mu(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}) \\ &= [\lambda\delta_{ij}N_{kk} + \mu(N_{ij} + N_{ji})]N_{ij} \\ &= 2\mu N_{ij}N_{ij} \\ &= 2\mu\frac{3}{2} \\ &= 3\mu \, . \end{aligned}$$

This fact has been used in in the derivation of (3.3).

The first order optimality conditions associated with the minimization problem (3.2) read

$$\begin{aligned} -\dot{\sigma}^{ef} + h[(1+C)\dot{\epsilon}^p + \tfrac{1}{2}B_i\dot{\epsilon}^p_{,i}] - \{h[A_{ij}\dot{\epsilon}^p_{,j} + \tfrac{1}{2}B_i\dot{\epsilon}^p]\}_{,i} &= 0 \quad \text{in } V \, , \\ h[A_{ij}\dot{\epsilon}^p_{,j} + \tfrac{1}{2}B_i\dot{\epsilon}^p]n_i &= \dot{\tau} \quad \text{on } S_T \, , \end{aligned}$$

which coincide with the flow rule of the FH model upon plastic loading. (See Appendix (A.27) for the derivation.)

Discretization in time

Since the plastic deformation is history dependent and irreversible, there is a need for the algorithm to update the plastic strain. In order to update the plastic strain, we should discretize the normality relation first. Regarding the stability issue, we adopt backward Euler method to discretize the normality relation and the internal

[1] Details are offered in Appendix (Lemma 1).

variables.

Assume that $[t^{(n)}, t^{(n+1)}]$ is a generic interval in time. The normalized flow direction $\mathbf{N}$ within this increment is defined by the deviatoric Cauchy stresses at the end of this increment, which means

$$N_{ij} = \frac{3}{2}\frac{S_{ij}^{(n+1)}}{\sigma^{ef,(n+1)}} \ . \tag{3.6}$$

The increment of the effective plastic strain is considered as an independent variable, and we define

$$\epsilon^{p,(n+1)} = \epsilon^{p,(n)} + \Delta\epsilon^p \ .$$

Discretizing the normality condition $\dot{\mathbf{E}}^p = \dot{\epsilon}^p\mathbf{N}$ with the flow direction defined in (3.6) leads to

$$E_{ij}^{p,(n+1)} = E_{ij}^{p,(n)} + \Delta\epsilon^p N_{ij} \ .$$

The generalized effective plastic strain is discretized by the following expression

$$\Lambda^{p,(n+1)} = \Lambda^{p,(n)} + \Delta\Lambda^p \ ,$$

where

$$\Delta\Lambda^p = \left((1+C)(\Delta\epsilon^p)^2 + A_{ij}\Delta\epsilon^p_{,i}\epsilon^p_{,j} + B_i\Delta\epsilon^p_{,i}\Delta\epsilon^p\right)^{\frac{1}{2}} \ .$$

It is worth emphasizing that since the model of Fleck and Hutchinson is an isotropic hardening model, the flow direction can be predicted by the strain increment as follows.

$$N_{ij} = \frac{3}{2}\frac{S_{ij}^{(n+1)}}{\sigma^{ef,(n+1)}} = \beta\mathrm{dev}(C_{ijkl}E_{kl}^{pre}) \ , \tag{3.7}$$

where

$$E_{kl}^{pre} = E_{kl}^{e,(n)} + \Delta E_{kl} \tag{3.8}$$

is the elastic strain predictor and β is a factor that normalizes $\mathbf{N}$.

With the preparation above, the functional for the variational constitutive update is discretized as

$$
\begin{aligned}
J_h(\Delta\epsilon^p; N_{ij}, \Delta E_{ij}) =& \frac{1}{2}\int_V C_{ijkl}(\Delta E_{ij} - \Delta\epsilon^p N_{ij})(\Delta E_{kl} - \Delta\epsilon^p N_{kl})\, dV \\
&+ \frac{1}{2}\int_V h(\Lambda^{p,(n+1)})(\Delta\Lambda^p)^2\, dV - \int_{S_T} \Delta\tau\Delta\epsilon^p\, dS
\end{aligned}
\tag{3.9}
$$

with $\Delta\tau = \tau^{(n+1)} - \tau^{(n)}$. The term $\int_{S_T} \dot{t}_i \dot{u}_i$ is not included since it is constant for the updates of the plastic strain.

Assuming that the strain increment $\Delta\mathbf{E}$ is prescribed, the increment of the effective plastic strain $\Delta\epsilon^p$ can be consistently obtained through the variation of the functional (3.9), i.e.

$$
\Delta\epsilon^p = arg \min_{\delta\epsilon^p} J_h(\delta\epsilon^p; N_{ij}, \Delta E_{ij}) \ . \tag{3.10}
$$

Being analogous with the continuous case, the first order optimality conditions of the minimization problem (3.9) yield

$$
\begin{aligned}
-\Delta\sigma^{ef} + \Delta\Sigma^Y - (\Delta m_i)_{,i} = 0 \quad &\text{in } V \\
\Delta m_i n_i = 0 \quad &\text{on } S\ ,
\end{aligned}
\tag{3.11}
$$

given the following definitions

$$
\left\{
\begin{array}{lcl}
\Delta\Sigma^Y &=& (\frac{1}{2}h'|_{\Lambda^{p,(n+1)}}\Delta\Lambda^p + h|_{\Lambda^{p,(n+1)}})((1+C)\Delta\epsilon^p + \frac{1}{2}B_i\Delta\epsilon^p_{,i}) \\
\Delta m_i &=& (\frac{1}{2}h'|_{\Lambda^{p,(n+1)}}\Delta\Lambda^p + h|_{\Lambda^{p,(n+1)}})(A_{ij}\Delta\epsilon^p_{,j} + \frac{1}{2}B_i\Delta\epsilon^p) \\
\Delta\sigma^{ef} &=& C_{ijkl}(\Delta E_{ij} - \Delta\epsilon^p N_{ij})N_{kl}\ .
\end{array}
\right.
\tag{3.12}
$$

These results are consistent with the results of the foregoing rate form in the sense that convergence to the corresponding rate formula can be achieved as the time-step approaches zero, provided that h' is finite. If the hardening function h is measured at $\Lambda^{p,(n)}$ rather than $\Lambda^{p,(n+1)}$ in the functional J_h, the first two definitions in (3.12) become

$$
\left\{
\begin{array}{lcl}
\Delta\Sigma^Y &=& h|_{\Lambda^{p,(n)}}((1+C)\Delta\epsilon^p + \frac{1}{2}B_i\Delta\epsilon^p_{,i}) \\
\Delta m_i &=& h|_{\Lambda^{p,(n)}}(A_{ij}\Delta\epsilon^p_{,j} + \frac{1}{2}B_i\Delta\epsilon^p)\ .
\end{array}
\right.
\tag{3.13}
$$

3.3 Finite element formulation

Assume that a solid body occupies a domain $V \subset \mathbb{R}^3$. The boundary of this body, S comprises two disjoint subsets S_T and S_U, such that $S = S_T \cup S_U$, $\phi = S_T \cap S_U$. S_T is the portion of the boundary where the traction $\mathbf{t}$ and the high order traction τ are specified, while S_U is the portion of the boundary where the displacement $\mathbf{u}$ and the effective plastic strain ϵ^p are specified. The initial boundary value problem can be stated as: *Find* $\mathbf{u}(\mathbf{x}, t)$ *and* $\epsilon^p(\mathbf{x}, t)$ *satisfying the initial conditions, equilibrium equations, compatibility equations and the constitutive equations* (2.19-2.40).

Assume that the deformation history of this solid body has been divided into a sequence of increments, $[t^{(n)}, t^{(n+1)}] \subset [0, T^f]$ is a generic increment in the deformation history and all the variables are known up to $t^{(n)}$. The incremental boundary value problem during this generic time interval can be stated as: *Find* $\mathbf{u}^{(n+1)}(\mathbf{x}, t)$ *and* $\epsilon^{p,(n+1)}(\mathbf{x}, t)$ *satisfying the equilibrium equations, compatibility equations and the constitutive equations below:*

Equilibrium equations:

$$T_{ij,j} = 0 \tag{3.14}$$

$$\Sigma - \sigma^{ef} - m_{i,i} = 0 \tag{3.15}$$

$$T_{ij} n_j = t_i \quad \text{on } S_T \tag{3.16}$$

$$m_i n_i = \tau \quad \text{on } S_T \tag{3.17}$$

Constitutive equations:

$$T_{ij} = C_{ijkl} E^e_{ij} \tag{3.18}$$

$$\Delta E^p_{ij} = \Delta \epsilon^p N_{ij} \tag{3.19}$$

$$N_{ij} = \frac{3}{2\sigma^{ef}} S_{ij} \tag{3.20}$$

$$S_{ij} = T_{ij} - \frac{1}{3} T_{kk} \tag{3.21}$$

$$\Delta\epsilon^p(\Sigma - \Sigma^Y) = 0 \tag{3.22}$$

$$\Delta\epsilon^p \geq 0 \tag{3.23}$$

$$\Sigma - \Sigma^Y \leq 0 \tag{3.24}$$

$$\Delta m_i = h(\Lambda^p)[A_{ij}\Delta\epsilon^p_{,j} + \frac{1}{2}B_i\Delta\epsilon^p] \tag{3.25}$$

$$\Delta\Sigma^Y = h(\Lambda^p)[(1+C)\Delta\epsilon^p + \frac{1}{2}B_i\Delta\epsilon^p_{,i}] \tag{3.26}$$

$$\Delta\Lambda^p = \left\{(\Delta\epsilon^p)^2 + A_{ij}\Delta\epsilon^p_{,i}\Delta\epsilon^p_{,j} + B_i\Delta\epsilon^p_{,i}\Delta\epsilon^p + C(\Delta\epsilon^p)^2\right\}^{\frac{1}{2}} \tag{3.27}$$

Compatibility equations:

$$E_{ij} = \frac{1}{2}(u_{i,j} + u_{j,i}) \tag{3.28}$$

$$E_{ij} = E^e_{ij} + E^p_{ij} \tag{3.29}$$

$$\sigma^{ef} = \sqrt{\frac{3}{2}S_{ij}S_{ij}} \tag{3.30}$$

$$u_i = u_i^S \quad \text{on } S_U \tag{3.31}$$

$$\epsilon^p = \epsilon^{p,S} \quad \text{on } S_U \tag{3.32}$$

Values at $t^{(n)}$ are taken as the initial conditions. Unless being specified, superscript $^{(n+1)}$ is omitted in the equations above. These equations are the discrete version of Eq (2.19-2.40) in Chapter 2, following directly from the discretization scheme in the previous section.

3.3.1 Computational framework

Since the deformation history of the solid body is divided into a sequence of increments, the key to building a numerical formulation is to construct an algorithm for solving the incremental boundary value problem within a generic time interval.

Our algorithm for a generic increment from $t^{(n)}$ to $t^{(n+1)}$ is described below:

1. Update the tractions and compute the external forces $\mathbf{F}^{ext}$. Initialize the displacements and the displacements increment, i.e. $\mathbf{u} := \mathbf{u}^{(n)}, \Delta\mathbf{u} := 0$.

2. Update the displacements, $\mathbf{u} := \mathbf{u} + \Delta\mathbf{u}$. Calculate the strain $\mathbf{E}$ and the flow direction $\mathbf{N}$.

3. Obtain the effective plastic strain ϵ^p and the stresses $\mathbf{T}$ through the variational constitutive update.

4. Calculate the internal force $\mathbf{F}^{int}$.

5. Check the force balance. Is $\|\mathbf{F}^{ext} - \mathbf{F}^{int}\|$ acceptable or not?

   - yes, $(\cdot)^{(n+1)} := (\cdot)$, exit iteration.
   - no, continue.

6. Calculate the consistent tangent matrix $\mathbf{K}$, which is the Jacobian of the system.

7. Obtain the displacement increment $\Delta\mathbf{u}$ by solving

$$\mathbf{K}\Delta\mathbf{u} = \mathbf{F}^{ext} - \mathbf{F}^{int} .$$

   Go to step 2.

The definitions and the expressions of terms $\mathbf{F}^{ext}$, $\mathbf{N}$, $\mathbf{F}^{int}$ and $\mathbf{K}$ will be provided in the next section.

3.3.2 Derivation of main equations

In this section, all the expressions of the terms that appear in our algorithm will be derived.

Assume φ_a is the shape function of the displacement field at node a and ψ_a is the shape function for the effective plastic strain field at node a. Then $\epsilon^p = \epsilon^p_a \psi_a$ and $u_i = u_{ia}\varphi_a$ with nodal unknowns ϵ^p_a and u_{ia}.

Flow direction:

$$N_{ij} = \beta \underbrace{(C_{ijkl}E^{pre}_{kl} - \frac{1}{3}\delta_{ij}C_{mmkl}E^{pre}_{kl})}_{=S^{pre}_{ij}} ,$$

where

$$\beta = \sqrt{\frac{3}{2}}(S^{pre}_{ij}S^{pre}_{ij})^{-\frac{1}{2}} , \quad E^{pre}_{kl} = E^{e,(n)}_{kl} + \Delta E_{kl} .$$

Internal force:

$$\begin{aligned} F^{int}_{ia} &= \int_V T_{ij}\varphi_{a,j}\, dx \\ &= \sum_e \int_e T_{ij}\varphi_{a,j}\, dx \end{aligned}$$

External force:

Assume there is no body force.

$$\begin{aligned} F^{ext}_{ia} &= \int_{S_T} t_i\varphi_a\, dS \\ &= \sum_e \int_{\partial e \cap S_T} t_i\varphi_a\, dS \end{aligned}$$

Variational constitutive updates:

The functional for the variational constitutive update is written in finite element formulation as follows.

$$\begin{aligned} J_h(\Delta\epsilon^p; \mathbf{u}) =& \frac{1}{2}\int_V C_{ijkl}[\Delta E_{ij} - \Delta\epsilon^p_a\psi_a N_{ij}][\Delta E_{kl} - \Delta\epsilon^p_b\psi_b N_{kl}]\, dx \\ &+ \frac{1}{2}\int_V h(\Lambda^p)(\Delta\Lambda^p)^2\, dx - \int_S \Delta\tau\Delta\epsilon^p_a\psi_a\, dS \end{aligned}$$

where

$$(\Delta\Lambda^p)^2 = (1+C)(\Delta\epsilon_a^p\psi_a)^2 + A_{ij}\Delta\epsilon_a^p\psi_{a,i}\Delta\epsilon_b^p\psi_{b,j} + B_i\Delta\epsilon_a^p\psi^{a,i}\Delta\epsilon_b^p\psi_b$$

and Λ^p has two choices, $\Lambda^{p,(n)}$ or $\Lambda^{p,(n+1)}$. We adopt $\Lambda^{p,(n)}$ because it will lead to a relatively simple formulation. The numerical examples in the next chapter show that the convergence is not affected by this choice.

We define $\mathbf{g}(\Delta\epsilon^p;\mathbf{u})$ as the derivative of $J_h(\Delta\epsilon^p;\mathbf{u})$ w.r.t. $\Delta\epsilon^p$.

$$\begin{aligned}
g_a =& \frac{\partial J_h}{\partial \Delta\epsilon_a^p} \\
=& \int_V C_{ijkl}[\Delta E_{kl} - \Delta\epsilon_b^p\psi_b N_{kl}][-\psi_a N_{ij}]\,dx \\
&+ \frac{1}{2}\int_V h[(1+C)2\Delta\epsilon_b^p\psi_b\psi_a + 2A_{ij}\Delta\epsilon_b^p\psi_{b,j}\psi_{a,i} \\
&+ B_i\psi_{a,i}\Delta\epsilon_b^p\psi_b + B_i\Delta\epsilon_b^p\psi_{b,i}\psi_a]\,dx - \int_S \Delta\tau\psi_a\,dS \\
=& \int_V -2\mu\Delta E_{kl}N_{kl}\psi_a + 3\mu\Delta\epsilon_b^p\psi_a\psi_b\,dx \\
&+ \frac{1}{2}\int_V h[(1+C)2\Delta\epsilon_b^p\psi_b\psi_a + 2A_{ij}\Delta\epsilon_b^p\psi_{b,j}\psi_{a,i} \\
&+ B_i\psi_{a,i}\Delta\epsilon_b^p\psi_b + B_i\Delta\epsilon_b^p\psi_{b,i}\psi_a]\,dx - \int_S \Delta\tau\psi_a\,dS
\end{aligned}$$

We define $\mathbf{H}(\Delta\epsilon_p;\mathbf{u})$ as the Hessian matrix of $J_h(\Delta\epsilon^p;\mathbf{u})$ w.r.t. $\Delta\epsilon^p$.

$$\begin{aligned}
H_{ab} =& \frac{\partial g_a}{\partial \Delta\epsilon_b^p} \\
=& \int_V C_{ijkl}N_{kl}N_{ij}\psi_a\psi_b\,dx \\
&+ \int_V h(1+C)\psi_a\psi_b + hA_{ij}\psi_{a,i}\psi_{b,j} + h\frac{B_i}{2}(\psi_{a,i}\psi_b + \psi_{b,i}\psi_a)\,dx \\
=& \int_V [3\mu + h(1+C)]\psi_a\psi_b + hA_{ij}\psi_{a,i}\psi_{b,j} + h\frac{B_i}{2}(\psi_{a,i}\psi_b + \psi_{b,i}\psi_a)\,dx\ .
\end{aligned} \tag{3.33}$$

The increment of the effective plastic strain $\Delta\epsilon^p$ can be obtained by solving a system of the linear equations

$$H_{ab}\Delta\epsilon^p_b = f_a$$

with $\mathbf{H}$ defined in (3.33) and

$$f_a = \int_V 2\mu\Delta E_{kl}N_{kl}\psi_a \, dx + \int_S \Delta\tau\psi_a \, dS \; .$$

Consistent tangent matrix:

The consistent tangent matrix is the Jacobian of the system. Using the consistent tangent matrix to solve the residual equations is essential for achieving a good convergence rate. In our specific algorithm, the consistent tangent matrix is defined by

$$\mathbf{K} = \frac{\partial \mathbf{F}^{int}}{\partial \mathbf{u}} \; .$$

The components of $\mathbf{K}$ have the expression:

$$\begin{aligned} K_{iajb} = \frac{\partial F^{int}_{ia}}{\partial u_{jb}} &= \frac{\partial}{\partial u_{jb}}(\int_V T_{im}\varphi_{a,m} \, dx) \\ &= \int_V \frac{\partial T_{im}}{\partial u_{jb}}\varphi_{a,m} \, dx \; . \end{aligned}$$

Since the Cauchy stresses

$$\begin{aligned} T_{im} &= C_{imst}(E_{st} - (E^{p,(n+1)}_{st}) \\ &= C_{imst}(E_{st} - (E^{p,(n)}_{st} + \Delta\epsilon^p N_{st})) \; , \end{aligned}$$

the derivative of the Cauchy stresses with respect to the nodal value of the displacements has the following expression

$$\frac{\partial T_{im}}{\partial u_{jb}} = C_{imst}[\underbrace{\frac{\partial E_{st}}{\partial u_{jb}}}_{=(I)} - \underbrace{\frac{\partial \Delta\epsilon^p}{\partial u_{jb}}}_{=(II)} N_{st} - \Delta\epsilon^p \underbrace{\frac{\partial N_{st}}{\partial u_{jb}}}_{=(III)}] \; . \qquad (3.34)$$

Terms (I) and (III) in (3.34) can be determined locally:

$$
\begin{aligned}
(I) = \frac{\partial E_{st}}{\partial u_{jb}} &= \frac{1}{2}\frac{\partial}{\partial u_{jb}}(u_{s,t} + u_{t,s}) \\
&= \frac{1}{2}\frac{\partial}{\partial u_{jb}}(u_{sa}\varphi_{a,t} + u_{ta}\varphi_{a,s}) \\
&= \frac{1}{2}(\delta_{js}\delta_{ab}\varphi_{a,t} + \delta_{jt}\delta_{ab}\varphi_{a,s}) \\
&= \frac{1}{2}(\delta_{js}\varphi_{b,t} + \delta_{jt}\varphi_{b,s}) \ .
\end{aligned}
\tag{3.35}
$$

$$
\begin{aligned}
(III) = \frac{\partial N_{st}}{\partial u_{jb}} &= \frac{\partial}{\partial u_{jb}}(\beta\, S_{st}^{pre}) \\
&= \frac{\partial \beta}{\partial u_{jb}} S_{st}^{pre} + \beta \frac{\partial}{\partial u_{jb}}(S_{st}^{pre}) \ .
\end{aligned}
\tag{3.36}
$$

Recalling the definitions of S_{st}^{pre} and the elastic strain predictor E_{kl}^{pre},

$$
\begin{cases}
S_{st}^{pre} = C_{stkl}E_{kl}^{pre} - \frac{1}{3}\delta_{st}C_{mmkl}E_{kl}^{pre} \\
E_{kl}^{pre} = E_{kl}^{e,(n)} + \Delta E_{kl} \ ,
\end{cases}
$$

$$
\begin{aligned}
\frac{\partial}{\partial u_{jb}}(S_{st}^{pre}) &= \frac{\partial}{\partial u_{jb}}(C_{stkl}E_{kl}^{pre} - \frac{1}{3}\delta_{st}C_{zzkl}E_{kl}^{pre}) \\
&= (C_{stkl} - \frac{1}{3}C_{zzkl}\delta_{st})\frac{\partial E_{kl}^{pre}}{\partial u_{jb}} \\
&= (C_{stkl} - \frac{1}{3}C_{zzkl}\delta_{st})\frac{\partial}{\partial u_{jb}}(E_{kl}^{e,(n)} + \Delta E_{kl}) \\
&= (C_{stkl} - \frac{1}{3}C_{zzkl}\delta_{st})\frac{\partial}{\partial u_{jb}}(E_{kl}^{e,(n)} + E_{kl} - E_{kl}^{(n)}) \\
&= (C_{stkl} - \frac{1}{3}C_{zzkl}\delta_{st})\frac{\partial}{\partial u_{jb}}(E_{kl}) \quad (\mathbf{E}^{e,(n)} \text{ and } \mathbf{E}^{(n)} \text{ are constants}) \\
&= (C_{stkl} - \frac{1}{3}C_{zzkl}\delta_{st})\frac{1}{2}(\delta_{jk}\varphi_{b,l} + \delta_{jl}\varphi_{b,k}) \ .
\end{aligned}
$$

Identity $\beta^2 = \frac{3}{2}(S_{kl}^{pre}S_{kl}^{pre})^{-1}$ implies

$$
2\beta\frac{\partial \beta}{\partial u_{jb}} = -\frac{3}{2}(S_{kl}^{pre}S_{kl}^{pre})^{-2}2S_{st}^{pre}\frac{\partial}{\partial u_{jb}}(S_{st}^{pre}) \ ,
$$

and consequently we can see

$$\frac{\partial \beta}{\partial u_{jb}} = -\frac{3}{2\beta}(S_{kl}^{pre} S_{kl}^{pre})^{-2} S_{st}^{pre} \frac{\partial}{\partial u_{jb}}(S_{st}^{pre}) ,$$

where now $\frac{\partial}{\partial u_{jb}}(S_{st}^{pre})$ has already been derived.

The term

$$(II) = \frac{\partial \Delta \epsilon^p}{\partial u_{jb}} = \frac{\partial \Delta \epsilon_c^p}{\partial u_{jb}} \psi_c$$

can not be determined locally, because obtaining $\Delta \epsilon^p$ from the variational constitutive update is equivalent to solving a partial differential equation including spatial derivatives throughout the domain.

The variational constitutive update together with the predictor step implies

$$\mathbf{g}(\Delta \epsilon^p(\mathbf{u}); \mathbf{u}) = 0,$$

for any tentative displacements $\mathbf{u}$. Since $\mathbf{g}$ as a function of $\mathbf{u}$ is constant, we have

$$\begin{aligned} 0 = \frac{\partial g_a}{\partial u_{jb}} &= \frac{\partial g_a}{\partial \Delta \epsilon_c^p} \frac{\partial \Delta \epsilon_c^p}{\partial u_{jb}} + \frac{\partial' g_a}{\partial' u_{jb}} \\ &= H_{ac} \frac{\partial \Delta \epsilon_c^p}{\partial u_{jb}} + \frac{\partial' g_a}{\partial' u_{jb}} \end{aligned}$$

with

$$\begin{aligned} \frac{\partial' g_a}{\partial' u_{jb}} &= \int_V -2\mu N_{kl} \psi_a \frac{\partial \Delta E_{kl}}{\partial u_{jb}} \, dx \\ &= \int_V -2\mu N_{kl} \psi_a \frac{\partial E_{kl}}{\partial u_{jb}} \, dx \\ &= \int_V -\mu N_{kl} \psi_a (\delta_{kj} \varphi_{b,l} + \delta_{lj} \varphi_{b,k}) \, dx \, . \end{aligned}$$

Consequently,

$$\frac{\partial \Delta \epsilon_c^p}{\partial u_{jb}} = -[\mathbf{H}^{-1}]_{ca} \frac{\partial' g_a}{\partial' u_{jb}} \, .$$

Finally, the expression of the consistent tangent matrix is obtained from the combination of the equations above:

$$
\begin{aligned}
K_{iajb} = &\int\limits_V C_{imjt}\varphi_{a,m}\varphi_{b,t}\,dx \\
&- \int\limits_V 2\mu\beta\Delta\epsilon^p(C_{imjl}\varphi_{a,m}\varphi_{j,l} - \frac{\lambda+2\mu}{3}\varphi_{a,i}\varphi_{b,j})\,dx \\
&- \int\limits_V \frac{8}{3}\mu\beta\Delta\epsilon^p N_{im}\varphi_{a,m}N_{jl}\varphi_{b,l}\,dx \\
&- 2\mu^2[\mathbf{H}^{-1}]_{\hat{c}\hat{a}}\int\limits_V N_{im}\varphi_{a,m}\psi_{\hat{c}}\,dx\int\limits_V N_{jl}\varphi_{b,l}\psi_{\hat{a}}\,dx\,.
\end{aligned}
\tag{3.37}
$$

The symmetry of $\mathbf{K}$ follows immediately from the expression (3.37), which is one advantage of the framework of variational constitutive updates as we can expect.

All the terms that appear in the computational framework have been clearly defined. In the next chapter, this numerical formulation will be tested through two benchmark examples.

Chapter 4

Numerical examples

Two examples in Fleck and Hutchinson's paper [12] are selected to examine the numerical formulation presented in Chapter 3. One of them is the shearing of a layer sandwiched by two rigid substrates; the other is wire torsion. Both examples are formulated as one-dimensional problems.

The hardening function h that appears in the expression of functional (3.9) results from a uniaxial tensile stress-strain curve, which is described by the Ramberg-Osgood relation

$$\frac{\epsilon}{\epsilon_0} = \frac{\sigma}{\sigma_0} + \left(\frac{\sigma}{\sigma_0}\right)^n \tag{4.1}$$

where $\sigma_0 = E\epsilon_0$ and E is Young's modulus. With the assumption of $\epsilon = \epsilon^e + \epsilon^p$, Eq (4.1) can be reformulated as

$$\sigma = \sigma_0 \left(\frac{\epsilon^p}{\epsilon_0}\right)^{\frac{1}{n}},$$

which yields

$$h(\Lambda^p) := \frac{\partial \sigma}{\partial \epsilon^p}|_{\Lambda^p} = \frac{E}{n}\left(\frac{\Lambda^p}{\epsilon_0}\right)^{\frac{1}{n}-1}. \tag{4.2}$$

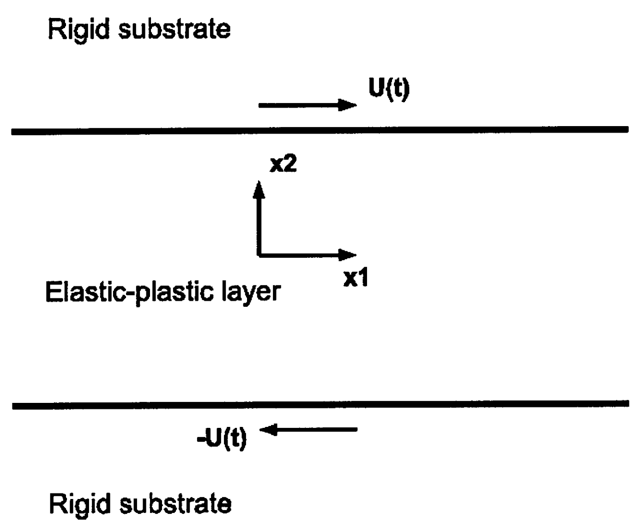

Figure 4-1: Sandwich layer: illustration

4.1 Shearing of a layer sandwiched by two rigid substrates

As illustrated in Fig (4-1), an infinite elastic-plastic layer sandwiched by two rigid substrates undergoes shearing displacements on its top and bottom surfaces.

Due to the geometry of this problem, the only primary unknowns are the displacement component $u_1(x_2, t)$ and the plastic strain component $\gamma^p(x_2, t) = 2E^p_{12}(x_2, t)$. Because the substrates are rigid, the dislocations inside of the layer can not exit; they will be blocked and thus pile up when they approach the boundaries. Within the continuum theory, this situation can be modeled as the plastic strain vanishes on the boundaries. Associated with these considerations, the boundary conditions for this problem are set as follows:

$$\begin{cases} u_1(L,t) = U(t), & \gamma^p(L,t) = 0 \\ u_1(-L,t) = -U(t), & \gamma^p(-L,t) = 0\,. \end{cases}$$

The effective plastic strain rate for this specific problem is

$$(\dot{\Lambda}^p)^2 = \frac{1}{3}(\dot{\gamma}^p)^2 + \frac{1}{3}l^2(\dot{\gamma}^{p'})^2 \tag{4.3}$$

with $\dot{\gamma}^{p'} = \frac{\partial \dot{\gamma}^p}{\partial x_2}$, which can be directly calculated from the definition (2.15). For this specific problem, the functional for the variational constitutive update (2.14) is reduced to

$$J(\dot{u}_i, \dot{\gamma}_p) = \frac{1}{2}\int_{-L}^{L} \mu(\dot{\gamma} - \dot{\gamma}^p)^2 + h(\Lambda^p)(\dot{\Lambda}^p)^2 \, dx_2$$

where $\dot{\gamma} = \frac{\partial \dot{u}_1}{\partial x_2}$ and $\dot{\Lambda}^p$ is defined in (4.3).

In the calculations, we have used the material parameters in Table (4.1), which match those used by Fleck an Hutchinson in their paper. The calculations are performed in one hundred increments in order to achieve a finial displacement of $10\epsilon_0 L$ at the boundaries. For each increment $[t^{(k)}, t^{(k+1)}]$, the displacement $U(t)$ at the

Table 4.1: Material parameters –1

Young's modulus	$E = 1.0\ \mathrm{N/m^2}$
Poisson ratio	$\nu = 0.3$
Ramberg-Osgood relation	$n = 5$ and $\epsilon_0 = 0.01$
Half width of the layer	$L = 1$ m
Length scales tested	$l/L \in [0, 0.05, 0.25, 0.5, 1]$

boundary is updated in the following way

$$U^{(k+1)} = U^{(k)} + 0.1\,\epsilon_0 L\ ,$$

where L is the half width of the layer, ϵ_0 is the parameter in the Ramberg–Osgood relation and $U^{(0)} = 0$. Both the displacement and the plastic shear strain are discretized by linear elements. Because the convergence analysis below shows that one hundred elements are sufficient to give converged results, we use one hundred elements to discretize the width of the layer when obtaining the data for Fig (4-2–4-5).

Fig (4-2–4-5) exhibit the final distributions of the displacement, the plastic shear strain, the shear stress and the generalized effective plastic strain fields from the simulations with different internal material length scales. In these figures, only the half width of the layer ($0 \leq x_2 \leq L$) is shown to emphasize the length scale effect.

From these figures, we can see that the displacement is linear only in the classical model. The stress in all cases remains uniform through the thickness, but its value increases significantly as the internal material length scale l increases. When l is small, there are distinct boundary layers in the distributions of the plastic shear strain. As l increases, the boundary layers become thick. Associated with the distributions of the plastic shear strain, the shape of the distribution of the generalized effective plastic strain is concave when l is small, and it becomes convex gradually as l increases. The boundary layers in the distributions of the plastic shear strain should be attributed to the boundary condition $\gamma^p(\pm L, t) = 0$. For comparison, results from the classical model (without essential boundary conditions for the plastic shear strain) are plotted

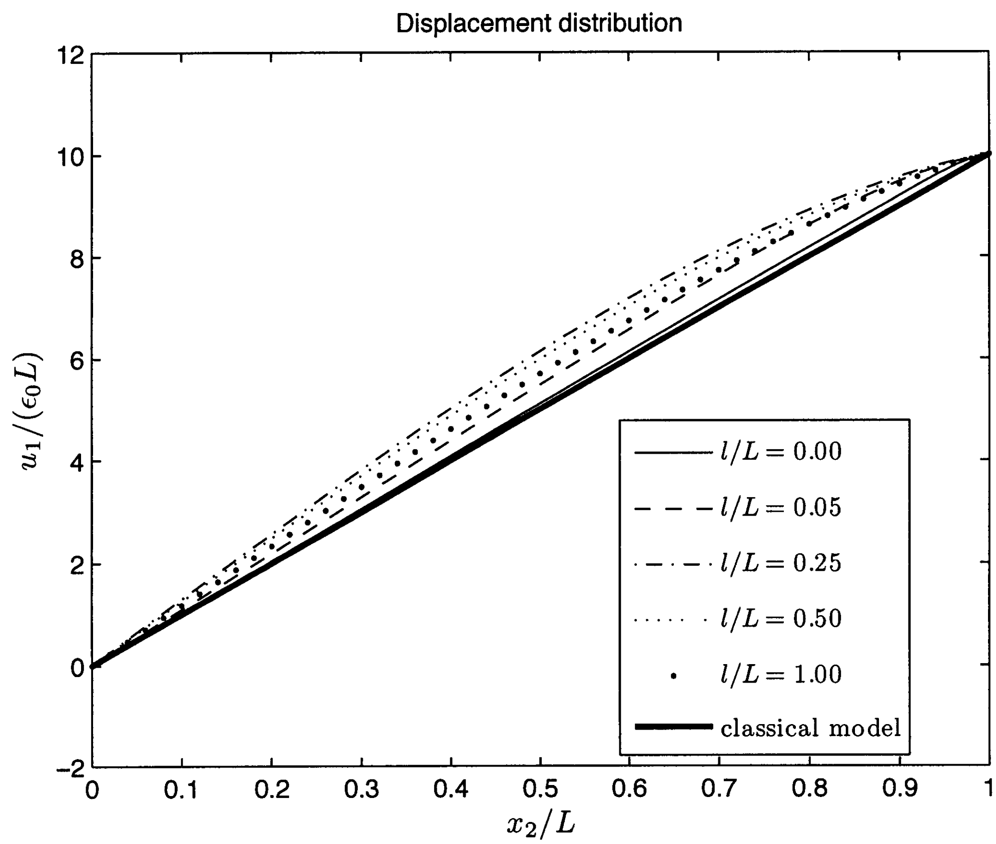

Figure 4-2: Sandwich layer: distribution of the displacement

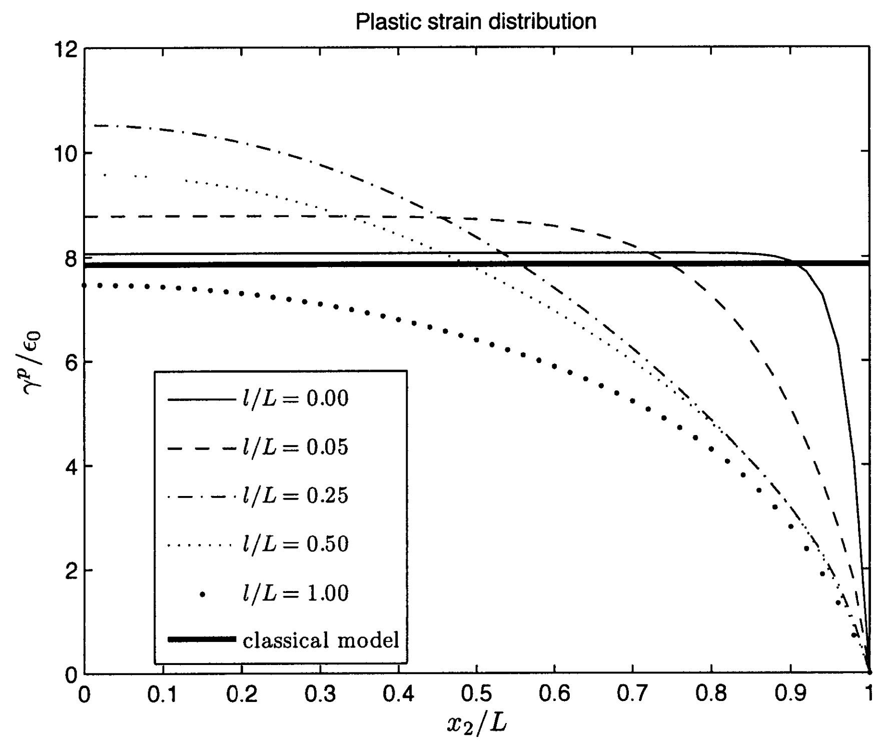

Figure 4-3: Sandwich layer: distribution of the plastic strain

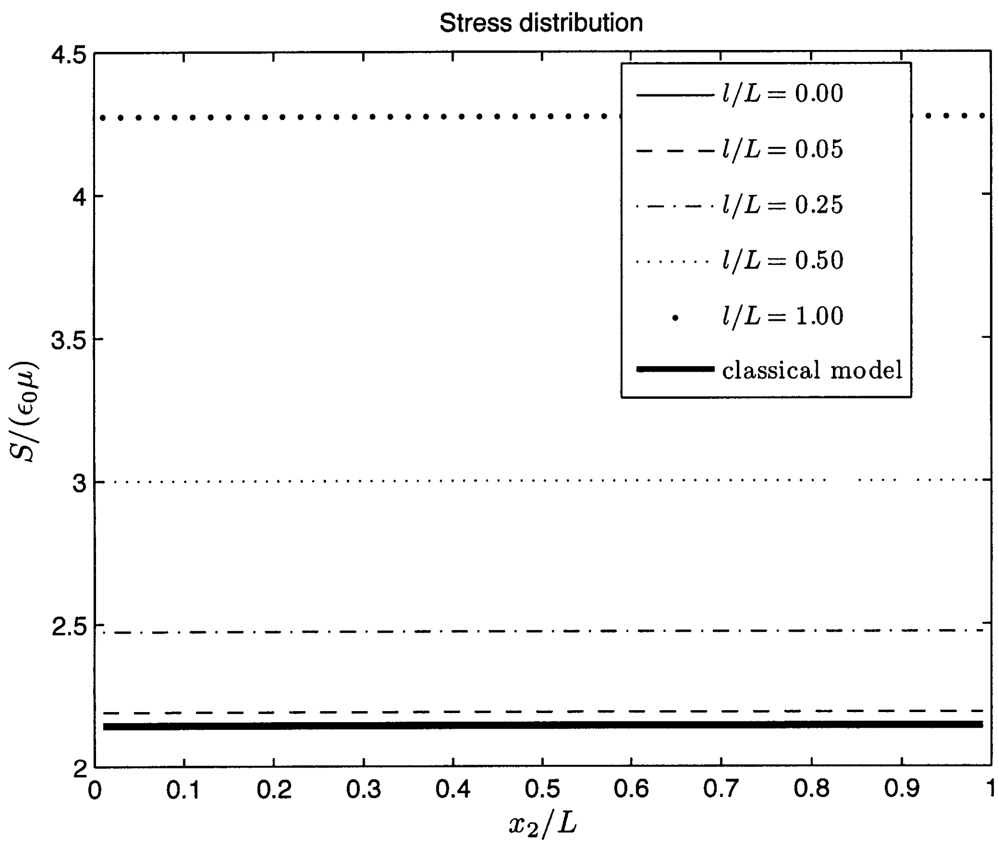

Figure 4-4: Sandwich layer: distribution of the shear stress

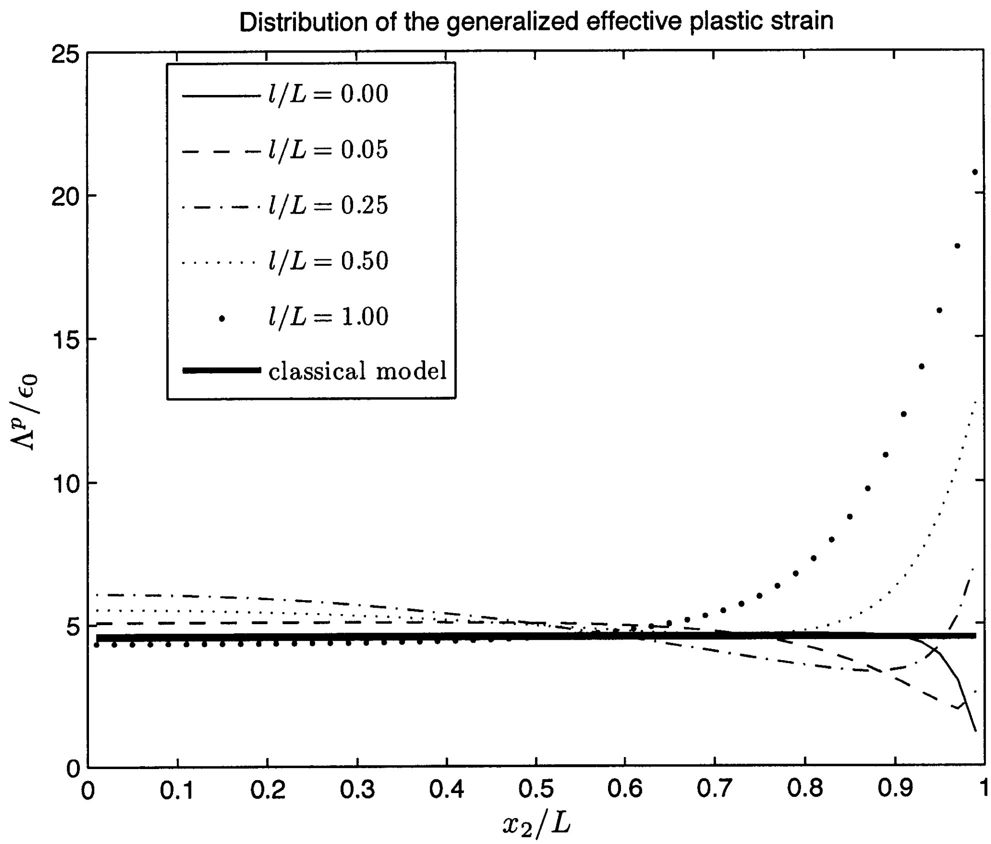

Figure 4-5: Sandwich layer: distribution of the generalized effective plastic strain

in these figures. As we can expect, the plastic shear strain in the classical model is uniform through the thickness. It is worth emphasizing that the flow rule of Fleck and Hutchinson's gradient model will degenerate to the classical J_2 flow theory as the internal material length scale approaches zero. The numerical formulation presented in this thesis provides the flexibility to impose boundary conditions on the effective plastic strain even when the internal material length scale is zero, while the effective plastic strain is not an independent variable in the classical model and no conditions should be imposed on it. Therefore we should impose the natural boundary conditions for the effective plastic strain in order to get the same result as the classical model predicts. In fact, recalling the flow rule for higher order stress (2.17)

$$\dot{m}_i = h[A_{ij}\dot{\epsilon}^p_{,j} + \frac{1}{2}B_i\dot{\epsilon}^p] ,$$

the natural boundary condition for the effective plastic strain in this specific problem can be written as

$$\begin{aligned} 0 = \dot{\tau} &= \dot{m}_i n_i \\ &= h\left(\frac{1}{3}l^2\dot{\gamma}^{p'}\right) . \end{aligned}$$

When $l = 0$, the natural boundary condition is automatically satisfied. This means no constraint is applied on the boundary for the plastic strain, which coincides with the situation in the classical local model.

In Fig (4-6), the evolution of the shear stress as the displacement increases is shown for different internal material length scales. As the length scale l increases, the material exhibits a stronger response. For the cases of $l = 0$, the stress histories of the simulation with essential boundary conditions and the simulation with natural boundary conditions (classical model) almost overlap. In Fig (4-7), we show a detail of these two stress histories, and we can find that the stress obtained from the simulation with $l = 0$ and the essential boundary conditions is greater than the stress obtained from the simulation with the classical model. This shows that essential boundary condition $\gamma^p = 0$ has an effect on strengthening even without the strain gradients, although this effect is relatively small.

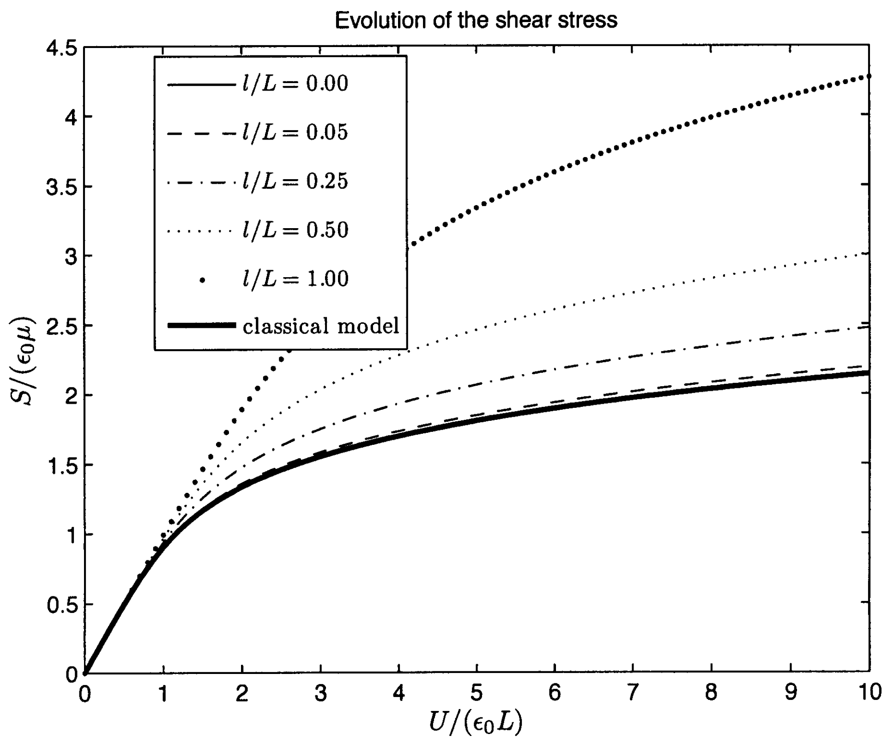

Figure 4-6: Sandwich layer: evolution of the shear stress

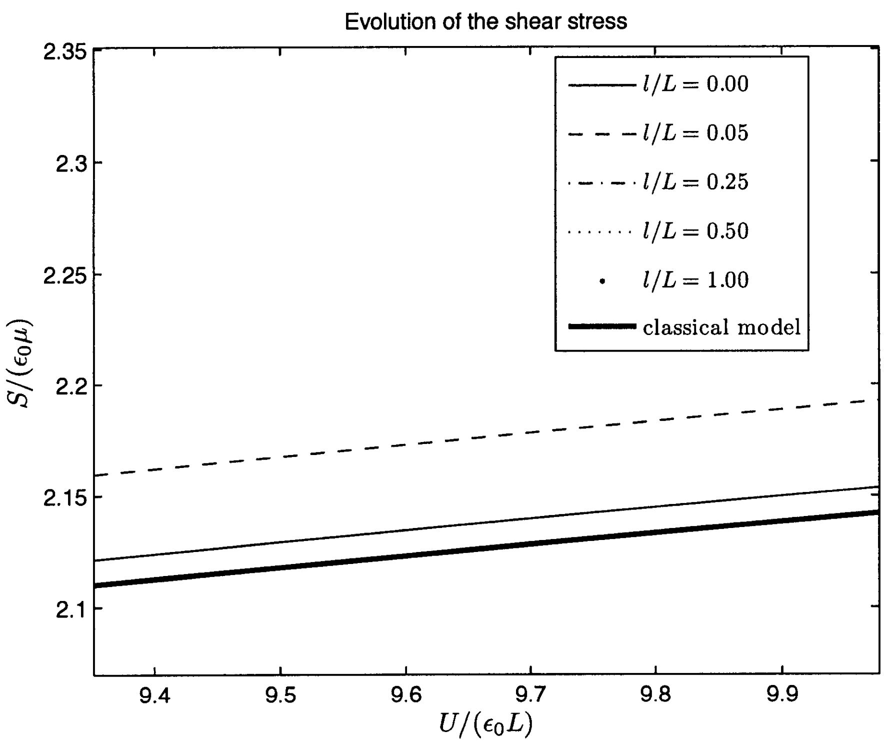

Figure 4-7: Sandwich layer: effect of the boundary conditions

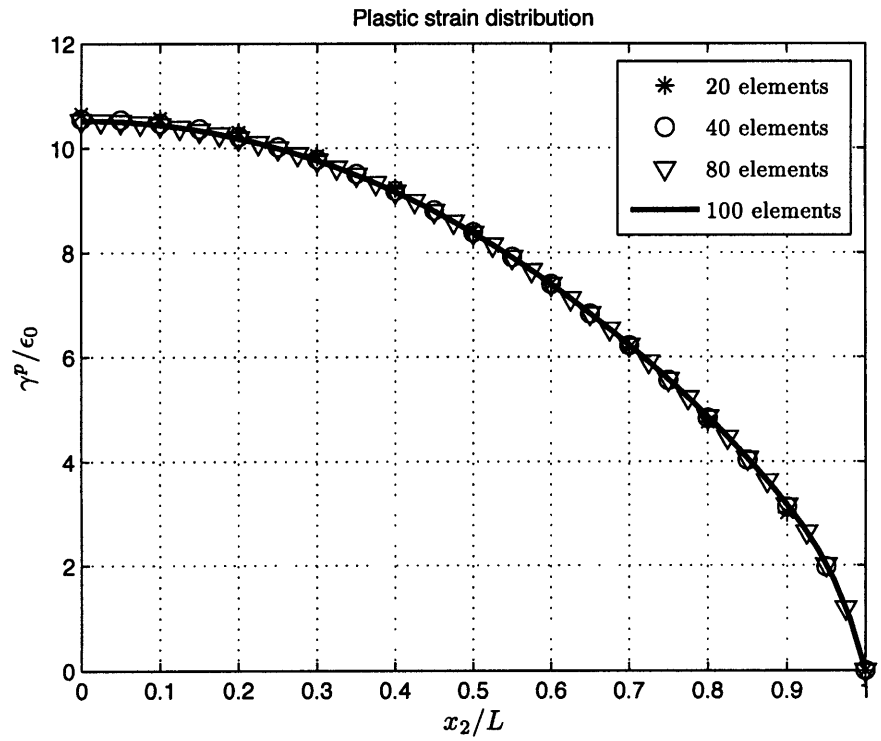

Figure 4-8: Sandwich layer: convergence of the plastic shear strain

The issue of convergence has also been examined. Since the exact solution is unknown, we conduct simultations with increasing number of elements until a satisfactory result is obtained, i.e. when there is no more visible change. The numerical results obtained from the simulations with twenty, forty, eighty and one hundred elements are used to test the convergence. In Fig (4-8) and Fig (4-9), the distributions of the plastic shear strain and the displacement are plotted respectively. Convergence is evident based on these two figures, and consequently the robustness of the numerical formulation is demonstrated. The data in these two figures correspond to internal material length scale $l = 0.25L$.

4.2 Wire torsion

Consider a cylindrical wire of radius R with the cylindrical coordinate system (r, θ, z). Assume that the wire is twisted monotonically. Then the total shear strain

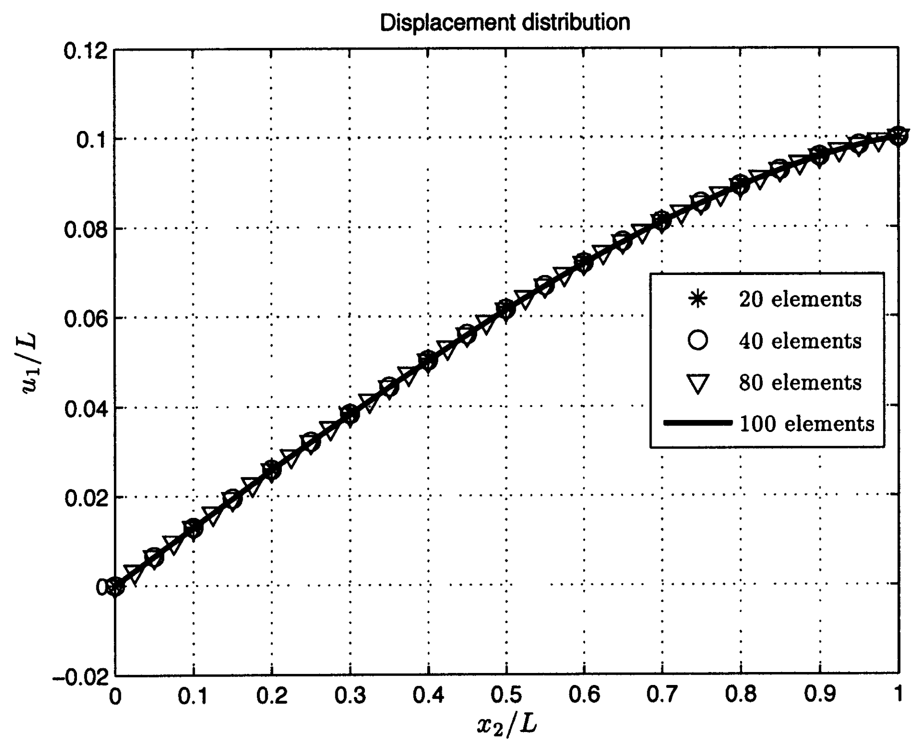

Figure 4-9: Sandwich layer: convergence of the displacement

is prescribed by

$$\gamma(r) = 2E_{\theta z}(r) = \alpha r \ ,$$

where α is the twist per unit length. Due to the geometry of this problem, the only non-zero variable is the plastic shear strain $\gamma^p(r) = 2E^p_{\theta z}$.

Assume that there is no constraint for the plastic flow at the outer boundary. Then, associated with this situation, the boundary condition at $r = R$ is set as

$$\tau(R, t) = 0 \ .$$

Also regarding the symmetry of this problem, the strain at the center of this cylindrical wire should vanish. Corresponding to this situation, the boundary condition at $r = 0$ reads

$$\gamma^p(0, t) = 0 \ .$$

Written in cylindrical coordinates, the rate of plastic shear strain tensor has the expression

$$\dot{\mathbf{E}}^p = \frac{1}{2}\dot{\gamma}^p(r)(\vec{e}_\theta\vec{e}_z + \vec{e}_z\vec{e}_\theta) \ ,$$

which results in the following nonzero gradients

$$\dot{E}^p_{\theta z,r} = \dot{E}^p_{z\theta,r} = \frac{1}{2}\dot{\gamma}^{p'} \ , \quad \dot{E}^p_{rz,\theta} = \dot{E}_{zr,\theta} = -\frac{1}{2}r^{-1}\dot{\gamma}^p \ .$$

Directly calculated from the definition (2.15), the generalized effective plastic strain rate for this specific problem has the expression

$$(\dot{\Lambda}^p)^2 = \frac{1}{3}(\dot{\gamma}^p)^2 + \frac{1}{6}l_1^2(\dot{\gamma}^{p'} - r^{-1}\dot{\gamma}^p)^2 + \frac{4}{3}l_2^2\left((\dot{\gamma}^{p'})^2 + r^{-1}\dot{\gamma}^{p'}\dot{\gamma}^p + r^{-2}(\dot{\gamma}^p)^2\right) \ ,$$

which can be reformulated as

$$(\dot{\Lambda}^p)^2 = d_1\dot{\gamma}_p^2 + d_2\dot{\gamma}_p\dot{\gamma}_p' + d_3\dot{\gamma}_p'^2$$

Table 4.2: Material parameters –2

Young's modulus	$E = 1.0\ \mathrm{N/m^2}$
Poisson ratio	$\nu = 0.3$
Ramberg-Osgood relation	$n = 5$ and $\epsilon_0 = 0.01$
Radius of the layer	$R = 1$ m
Length scales tested	$(\frac{l_1}{R}, \frac{l_2}{R}) \in \{(0,0), (.02,.2), (2,.2), (.05,.5), (5,.5), (.2,.1)\}$

with

$$\begin{cases} d_1 &= \frac{1}{3} + (\frac{1}{6}l_1^2 + \frac{4}{3}l_2^2)r^{-2} \\ d_2 &= (-\frac{1}{3}l_1^2 + \frac{4}{3}l_2^2)r^{-1} \\ d_3 &= \frac{1}{6}l_1^2 + \frac{4}{3}l_2^2 \ . \end{cases}$$

In this problem, the functional for the variational constitutive update (2.14) is reduced to

$$J(\dot{\gamma}^p) = \frac{1}{2}\int_0^R [\mu(\dot{\alpha}r - \dot{\gamma}^p)^2 + h(\Lambda^p)(\dot{\Lambda}^p)^2] 2\pi r \, dr \ .$$

Since the strain field is imposed externally, solving this problem purely examines the performance of the variational constitutive update. In the calculations, we have used the material parameters listed in Table (4.2), which match those used by Fleck and Hutchinson. The calculation is performed by five hundred increments in order to achieve the final strain of $10\epsilon_0$. Within each increment $[t^{(k)}, t^{(k+1)}]$, the twist per unit length is updated in the following way

$$\alpha^{(k+1)} = \alpha^{(k)} + 0.1\,\epsilon_0/R \ ,$$

where ϵ_0 is a parameter in the Ramberg–Osgood relation, R is the radius of the wire and $\alpha^{(0)} = 0$. The plastic shear strain is discretized in linear elements. One hundred elements are used to discretize the radius of the wire except for the calculation for demonstrating the convergence.

Final distributions of the plastic shear strain are collected in Fig (4-10). It is clear that the internal length scales affect the slope of the plastic shear strain at $r = R$.

This fact can be explained using the flow rule for higher order stress (2.17)

$$\dot{m}_i = h[A_{ij}\dot{\epsilon}^p_{,j} + \frac{1}{2}B_i\dot{\epsilon}^p] \ .$$

Combined with the natural boundary condition

$$\dot{m}_i n_i = \dot{r} = 0$$

at $r = R$, the flow rule for this specific problem reads

$$\begin{aligned} 0 &= d_3\dot{\gamma}^{p'} + \frac{1}{2}d_2\dot{\gamma}^p \\ &= (\frac{1}{6}l_1^2 + \frac{4}{3}l_2^2)\dot{\gamma}^{p'} + \frac{1}{2}(-\frac{1}{3}l_1^2 + \frac{4}{3}l_2^2)r^{-1}\dot{\gamma}^p \ . \end{aligned}$$

If $l_1 = 2l_2 \neq 0$, $\dot{\gamma}^{p'} = 0$ will be enforced. If l_1 dominates,

$$\dot{\gamma}^{p'} - r^{-1}\dot{\gamma}^p = 0$$

will be approximately enforced, and the slope $\dot{\gamma}^{p'} \approx r^{-1}\dot{\gamma}^p > 0$, since $\dot{\gamma}^p > 0$ at $r = R$. If l_2 dominates,

$$\dot{\gamma}^{p'} + \frac{1}{2}r^{-1}\dot{\gamma}^p = 0$$

will be approximately enforced, and the slope $\dot{\gamma}^{p'} \approx -\frac{1}{2}r^{-1}\dot{\gamma}^p < 0$, since $\dot{\gamma}^p > 0$ at $r = R$. The results shown in Fig (4-10) are consistent with this limiting behavior. The evolution of the torque is collected in Fig (4-11). In this figure, we can see that as l_2 increases, the material exhibits a stronger response. In addition, we can find that l_1 has only a slight influence on the torque-twist relation. In Fig (4-11), torque T is calculated through the following formula

$$\begin{aligned} T &= \int_0^R \int_0^{2\pi} rT_{z\theta}r \ drd\theta \\ &= \int_0^R T_{z\theta}2\pi r^2 \ dr \end{aligned}$$

with shear stress $T_{z\theta} = \mu(\alpha r - \gamma^p)$.

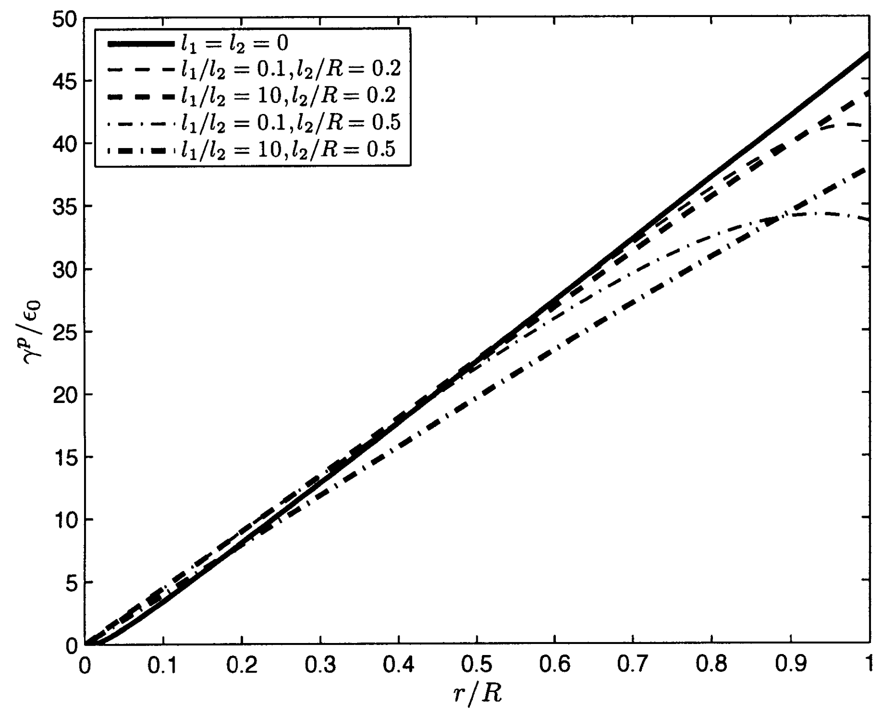

Figure 4-10: Wire torsion: distribution of the plastic shear strain

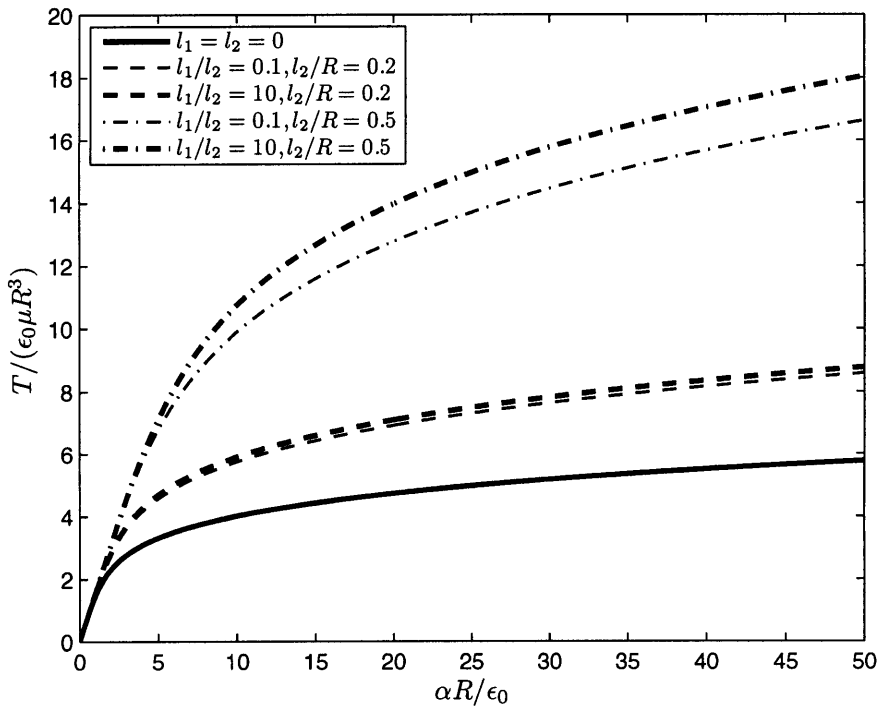

Figure 4-11: Wire torsion: torque v.s. twist

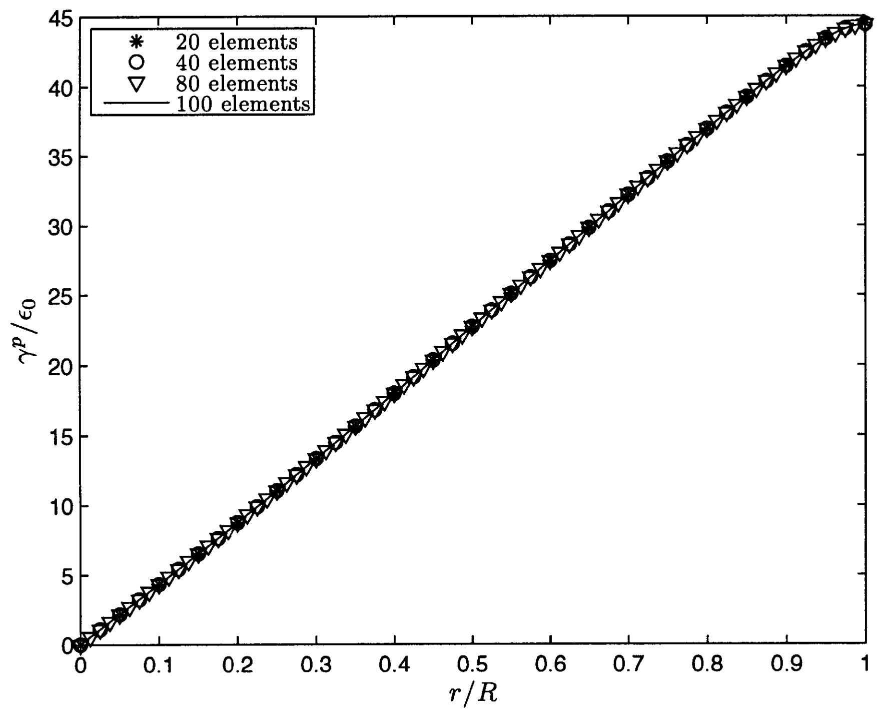

Figure 4-12: Wire torsion: distribution of the plastic shear strain

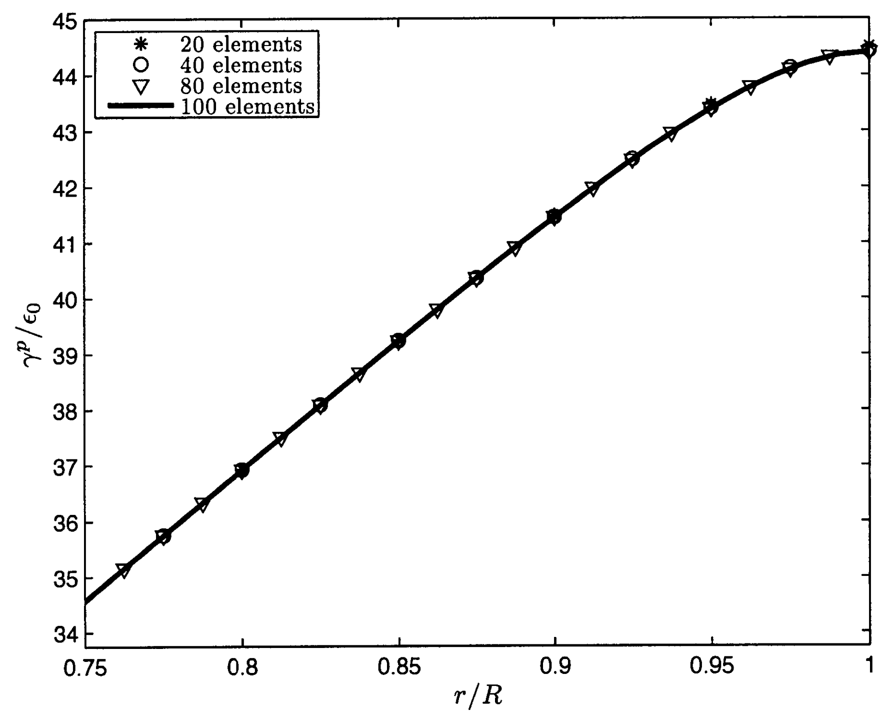

Figure 4-13: Wire torsion: zoom-in of Fig (4-12)

The issue of convergence has also been examined. Since the exact solution is unknown, we conduct simulations with increasing number of elements until a satisfactory result is obtained, i.e. when there is no visible change. The numerical results from the simulations with twenty, forty, eighty and one hundred elements are used to examine the convergence. In Fig (4-12) and Fig (4-13), the distributions of the plastic shear strain are plotted. Convergence is evident based on these two figures; consequently the robustness of the numerical formulation is demonstrated. The data in these two figures correspond to internal material length scales $l_1 = 0.2R$ and $l_2 = 0.1R$.

Chapter 5

Discussion and conclusions

5.1 Fleck and Hutchinson's model revisited

In 2009, Evans and Hutchinson assessed the model of Nix and Gao and also the model of Fleck and Hutchinson (FH model) using the simple bending test as an example [9]. Two main conclusions were drawn in their paper. One conclusion is that the expression of the generalized effective plastic strain rate in Fleck and Hutchinson's model (2.15)

$$\dot{\Lambda}^p = \left\{(\dot{\epsilon}^p)^2 + A_{ij}\dot{\epsilon}^p_{,i}\dot{\epsilon}^p_{,j} + B_i\dot{\epsilon}^p_{,i}\dot{\epsilon}^p + C(\dot{\epsilon}^p)^2\right\}^{\frac{1}{2}}$$

should be replaced by the following expression

$$\dot{\Lambda}^p = \dot{\epsilon}^p + [A_{ij}\dot{\epsilon}^p_{,i}\dot{\epsilon}^p_{,j} + B_i\dot{\epsilon}^p_{,i}\dot{\epsilon}^p + C(\dot{\epsilon}^p)^2]^{\frac{1}{2}} \ , \tag{5.1}$$

because the resulting model will 'correlate with the well-established square root size scaling trends found in hardness and other tests'. The other conclusion is that the variational structure of Fleck and Hutchinson's model should be retained because of its flexibility to impose boundary conditions associated with the effective plastic strain.

Although the new definition of the generalized effective strain rate (5.1) extends the ability of the FH model to match a wide range of the experimental data, it also breaks the mathematical structure of the original FH model. Rates $(\dot{\mathbf{u}}, \dot{\epsilon}^p)$ that minimize the functional (2.14)

$$I(\dot{\mathbf{u}}, \dot{\epsilon}^p) = \frac{1}{2}\int_V C_{ijkl}(\dot{E}_{ij} - \dot{\epsilon}^p N_{ij})(\dot{E}_{kl} - \dot{\epsilon}^p N_{kl}) + h(\Lambda^p)(\dot{\Lambda}^p)^2 \, dV - \int_{S_T} \dot{t}_i \dot{u}_i + \dot{\tau}\dot{\epsilon}^p \, dS \, .$$

may not be smooth. The first numerical example in the previous chapter, shearing of a layer sandwiched by two substrates, is a good example to explain this smoothness issue. In the original FH model, the generalized effective plastic strain rate is

$$(\dot{\Lambda}^p)^2 = \frac{1}{3}(\dot{\gamma}^p)^2 + \frac{1}{3}l^2(\dot{\gamma}^{p'})^2 \, .$$

In the improved model, it reads

$$\dot{\Lambda}^p = \frac{1}{\sqrt{3}}\dot{\gamma}^p + \frac{l}{\sqrt{3}}|\dot{\gamma}^{p'}| \, .$$

The higher order stress corresponding to this generalized effective plastic strain rate is

$$\dot{m} = \frac{h}{\sqrt{3}}\left(l\dot{\gamma}^p \frac{\dot{\gamma}^{p'}}{|\dot{\gamma}^{p'}|} + l^2\dot{\gamma}^{p'}\right) \, . \tag{5.2}$$

(See Appendix (A.27) for the derivation.) Due to the symmetry of this problem, the plastic shear strain rate should be an even function, which means

$$\dot{\gamma}^p(x_2, t) = \dot{\gamma}^p(-x_2, t), \quad \text{for } 0 < x_2 \le L \, .$$

If the plastic strain gradient $\dot{\gamma}^{p'}$ exists and is continuous,

$$\dot{\gamma}^{p'}(x_2, t) = -\dot{\gamma}^{p'}(-x_2, t), \quad \text{for } 0 < x_2 \le L \, ;$$

consequently at the center of the layer

$$\dot{\gamma}^{p'}(0, t) = 0 \, .$$

Again due to the symmetry of this problem, the plastic shear strain rate is always positive at the center of the layer, which implies that

$$\dot{\gamma}^p \frac{\dot{\gamma}^{p'}}{|\dot{\gamma}^{p'}|}$$

is ill-posed at the center of the layer. As a result, the higher order stress defined in (5.2) is ill-posed too, and the equilibrium equation (A.27) that involves the divergence of the higher order stresses

$$\dot{\Sigma}^Y - \dot{\sigma}^{ef} - \dot{m}_{i,i} = 0$$

is not well defined. All these issues suggest that the assumption of the continuity of $\dot{\gamma}^{p'}$ must be abandoned in the improved model.

In 2009, Fleck and Willis proposed a strain gradient plasticity model that can also be considered as an improvement of the original Fleck and Hutchinson's model [14]. In their work, the definition of the generalized effective plastic strain (2.15) is retained, but the generalized effective stress is redefined in order to satisfy the thermodynamics requirement. In the original FH model, the generalized effective stress Σ is exactly the work-conjugate to ϵ^p, while in the model of Fleck and Willis, it comprises both the work-conjugate to ϵ^p and the work-conjugate to $\epsilon^p_{,i}$. Assume that the generalized effective plastic strain rate is defined by the expression

$$\dot{\Lambda}^p = \left\{(\dot{\epsilon}^p)^2 + A_{ij}\dot{\epsilon}^p_{,i}\dot{\epsilon}^p_{,j} + B_i\dot{\epsilon}^p_{,i}\dot{\epsilon}^p + C(\dot{\epsilon}^p)^2\right\}^{\frac{1}{2}} .$$

Corresponding to this definition, the generalized effective stress in Fleck and Willis' model is defined by

$$\Sigma = \left([\bar{\mathbf{A}}^{-1}]_{ij} r_i r_j\right)^{\frac{1}{2}}$$

with

$$\bar{\mathbf{A}} = \begin{bmatrix} A_{11} & A_{12} & A_{13} & \frac{1}{2}B_1 \\ A_{21} & A_{22} & A_{23} & \frac{1}{2}B_2 \\ A_{31} & A_{32} & A_{33} & \frac{1}{2}B_3 \\ \frac{1}{2}B_1 & \frac{1}{2}B_2 & \frac{1}{2}B_3 & 1+C \end{bmatrix}$$

and

$$\mathbf{r} = [m_1,\ m_2,\ m_3,\ Q]^{\tau} \ ,$$

where $\mathbf{m}$ is the higher order stresses and Q is the work-conjugate to the effective plastic strain ϵ^p. Associated with the new definition of the generalized effective stress, Fleck and Willis presented the following normality relations

$$\dot{\epsilon}^p_{,i} = \dot{\Lambda}^p \frac{\partial \Sigma}{\partial r_i} = \frac{\dot{\Lambda}^p}{\Sigma}\left([\bar{\mathbf{A}}^{-1}]_{ij} r_j\right) \tag{5.3}$$

and

$$\dot{\epsilon}^p = \dot{\Lambda}^p \frac{\partial \Sigma}{\partial r_4} = \frac{\dot{\Lambda}^p}{\Sigma}\left([\bar{\mathbf{A}}^{-1}]_{4j} r_j\right) \ . \tag{5.4}$$

With these normality relations, the non-negativeness of the plastic work is guaranteed, since the plastic work

$$Q\dot{\epsilon}^p + m_i \dot{\epsilon}^p_{,i} = \frac{\dot{\Lambda}^p}{\Sigma}\left([\bar{\mathbf{A}}^{-1}]_{ij} r_i r_j\right) = \dot{\Lambda}^p \Sigma \geq 0 \ .$$

Another feature of Fleck and Willis' model is that the effect of interface is considered. They believed that both the jump in the plastic strain and the increment in the mean plastic strain at the interfaces induce dissipation and consequently strengthen the response of the material.

5.2 Other problems with coupled fields

The initial boundary value problem from strain gradient isotropic plasticity theories is one specific example of the problems with coupled fields. In the strain gradient isotropic plasticity theories, the displacement and the effective plastic strain fields are coupled. There are also some other problems involving the coupled fields, such as the thermal elastic models, the thermal plastic models and the gradient damage models.

5.2.1 Gradient damage model

The initial boundary value problem from the strain gradient damage theory is another example of the problems with coupled fields [31]. In particular, there are some similarities between the governing equations of the strain gradient damage theory and the governing equations of the strain gradient isotropic plasticity theories presented in this thesis.

The displacement field $\mathbf{u}$ and a scale field $\bar{\epsilon}$, the equivalent strain, are two coupled fields in the strain gradient damage model presented in [31]. The governing equations of this damage model are listed below.

Equilibrium equation:

$$T_{ij,j} + f_i = 0 \ ,$$

where $\mathbf{T}$ is the Cauchy stress tensor and $\mathbf{f}$ is the body force.

Constitutive equations:

$$T_{ij} = (1 - D(\kappa))\, C_{ijkl} E_{kl} \tag{5.5}$$

$$\dot{\kappa}(\bar{\epsilon} - \kappa) = 0 \tag{5.6}$$

$$\dot{\kappa} \geq 0 \tag{5.7}$$

$$\bar{\epsilon} - \kappa \leq 0 \tag{5.8}$$

$$\bar{\epsilon} = \epsilon^{eq} + c^2 \nabla^2 \epsilon^{eq} \tag{5.9}$$

$$D(\kappa) = \begin{cases} 0 & \text{if } \kappa \leq \kappa^0 \\ 1 - \frac{\kappa^0(\kappa^c - \kappa)}{\kappa(\kappa^c - \kappa^0)} & \text{if } \kappa^0 < \kappa < \kappa^c \\ 1 & \text{if } \kappa \geq \kappa^c \end{cases} \tag{5.10}$$

where ϵ^{eq} is an invariant of the local strain tensor, κ is the maximum positive value of the equivalent strain in the history, c is an internal material length scale and $D(\kappa)$ describes the influence of the maximum equivalent strain κ on the elastic response. When κ is less than κ^0, the response of the material is fully elastic. As κ increases, the damage develops and the elastic response is weakened by a factor of $D(\kappa)$. Finally, when κ reaches κ^c, the elastic response is no longer valid, and the material is totally damaged.

The strain gradient damage model above is an elasticity model, and in principle $\bar{\epsilon}$ can be expressed explicitly in term of the displacement $\mathbf{u}$ once the expression of the ϵ^{eq} is provided. Nonetheless, with the structure rather than the dimension in consideration, we can find that ϵ^{eq}, $\bar{\epsilon}$ and κ correspond to ϵ^{p}, Σ and Σ^{Y} respectively.

5.3 Conclusions

A numerical formulation based on the framework of the variational constitutive update has been presented to solve the initial boundary value problem from the strain gradient isotropic plasticity theories. Various strain gradient isotropic plasticity models have been summarized and compared in Chapter 2. Among these models, Fleck and Hutchinson's model is adopted by this numerical formulation because it has a relatively simple form and is sufficiently general. The numerical formulation based on the variational constitutive update is constructed and compared to the current numerical methods in Chapter 3. The robustness of this numerical formulation is verified through the finite element implementation on the benchmark examples in Chapter 4.

As discussed at the beginning of this chapter, the model of Fleck and Hutchinson has been improved by the two authors separately. It can be a possible extension of current work to apply the numerical formulation for these improved models. Implementing this numerical formulation to other coupled fields problems, such as the gradient damage model, is another possible extension. There is also some other possible future work, such as applying the current numerical formulation for three-dimensional problems, testing the combinations of the finite element spaces of the displacement and the effective plastic strain fields, and extending the current numerical formulation for the large deformation and dynamic problems.

The long-term objective of this work is to construct a robust and efficient computational framework for the strain gradient crystal plasticity theories, especially for the investigation on the tissue level problems. The experiences and knowledges gained from constructing the numerical formulation for the strain gradient isotropic plasticity theories provide a solid foundation for the author to move towards the long-term objective.

Appendix A

A.1 Expression of the generalized effective plastic strain rate

The generalized effective plastic strain rate in the gradient model of Fleck and Hutchinson has the expression

$$(\dot{\Lambda}^p)^2 = (\dot{\epsilon}^p)^2 + A_{ij}\dot{\epsilon}^p_{,i}\dot{\epsilon}^p_{,j} + B_i\dot{\epsilon}^p_{,i}\dot{\epsilon}^p + C(\dot{\epsilon}^p)^2 \ ,$$

where A_{ij}, B_i and C depend on three internal material length scales. In this section, this expression will be explained.

The generalized effective plastic strain rate $\dot{\Lambda}^p$ comprises the plastic strain rate $\dot{\mathbf{E}}^p$ and its gradients. Perhaps the most intuitive way to define $\dot{\Lambda}^p$ is to adopt the expression below:

$$\begin{aligned}(\dot{\Lambda}^p)^2 &= \frac{2}{3}(\dot{E}^p_{ij}\dot{E}^p_{ij}) + l^2(\dot{E}^p_{ij,k}\dot{E}^p_{ij,k}) \\ &= (\dot{\epsilon}^p)^2 + l^2(\dot{E}^p_{ij,k}\dot{E}^p_{ij,k}) \ .\end{aligned} \tag{A.1}$$

Eq (A.1) does include the contribution from the gradients of the plastic strain, however it only contains one parameter. In order to provide more flexibility for data fitting, it is natural to consider other invariants in addition to $\dot{E}^p_{ij,k}\dot{E}^p_{ij,k}$ and to introduce more internal material length scales. Define

$$\rho_{ijk} = \dot{E}^p_{ij,k} \ .$$

In general, there are twelve independent invariants of degree two for a third order tensor, which can be written as follows:

$$\rho_{ijk}\rho_{ijk},\ \rho_{ijk}\rho_{ikj},\ \rho_{ijk}\rho_{jik},\ \rho_{ijk}\rho_{jki},\ \rho_{ijk}\rho_{kij},\ \rho_{ijk}\rho_{kji}\ , \tag{A.2}$$

and

$$\rho_{iij}\rho_{jkk},\ \rho_{iij}\rho_{kjk},\ \rho_{iij}\rho_{kkj},\ \rho_{iji}\rho_{jkk},\ \rho_{iji}\rho_{kjk},\ \rho_{jii}\rho_{jkk}\ . \tag{A.3}$$

In the strain gradient plasticity model, $\rho_{ijk} = \dot{E}^p_{ij,k}$ is not a general third order tensor. In the model of Fleck and Hutchinson, it is assumed that the plastic deformation is incompressible, and the strain rate $\dot{\mathbf{E}}^p$ is symmetric. These assumptions can be expressed mathematically as

$$\rho_{iik} = 0, \quad \rho_{ijk} = \rho_{jik}\ . \tag{A.4}$$

Because of these assumptions, the number of the invariants is reduced to three. These invariants are

$$\rho_{ijk}\rho_{ijk},\ \rho_{ijk}\rho_{ikj},\ \rho_{jii}\rho_{jkk}\ . \tag{A.5}$$

Therefore, we can assign three parameters, and define the generalized effective plastic strain as follows:

$$(\dot{\Lambda}^p)^2 = (\dot{\epsilon}^p)^2 + c_1\rho_{ijk}\rho_{ijk} + c_2\rho_{ijk}\rho_{ikj} + c_3\rho_{jii}\rho_{jkk}\ , \tag{A.6}$$

where c_1, c_2, c_3 are three parameters with the dimension of the square of length. Expression (A.6) is already general, however it is not satisfying because the invariant $\rho_{ijk}\rho_{ikj}$ may take negative value, and the necessary condition for

$$c_1\rho_{ijk}\rho_{ijk} + c_2\rho_{ijk}\rho_{ikj} + c_3\rho_{jii}\rho_{jkk} \geq 0$$

is not clear. In order to simplify the requirement for choosing the internal material length scales, Fleck and Hutchinson adopted an orthogonal decomposition (Details can be found in [12])

$$\rho_{ijk} = \rho^{(1)}_{ijk} + \rho^{(2)}_{ijk} + \rho^{(3)}_{ijk} \; ,$$

and defined the generalized effective plastic strain as follows:

$$(\dot{\Lambda}^p)^2 = (\dot{\epsilon}^p)^2 + L_1^2 \rho^{(1)}_{ijk}\rho^{(1)}_{ijk} + 4L_2^2 \rho^{(2)}_{ijk}\rho^{(2)}_{ijk} + \frac{8}{3}L_3^2 \rho^{(3)}_{ijk}\rho^{(3)}_{ijk} \; . \tag{A.7}$$

Since $\rho_{ijk} = \dot{E}^p_{ij,k} = (\dot{\epsilon}^p N_{ij})_{,k} = \dot{\epsilon}^p_{,k} N_{ij} + \dot{\epsilon}^p N_{ij,k}$, the expression (A.7) can be reformulated as

$$(\dot{\Lambda}^p)^2 = (\dot{\epsilon}^p)^2 + A_{ij}\dot{\epsilon}^p_{,i}\dot{\epsilon}^p_{,j} + B_i \dot{\epsilon}^p_{,i}\dot{\epsilon}^p + C(\dot{\epsilon}^p)^2 \; . \tag{A.8}$$

In the definition above, parameters A_{ij}, B_i, C have the following expressions.

$$\begin{aligned}
A_{ij} = \;& L_1^2(\tfrac{1}{2}\delta_{ij} + \tfrac{2}{5}N_{ip}N_{jp}) + e_{pir}N_{qr}(\hat{L}_2^2 e_{pjv}N_{qv} + \hat{L}_3^2 e_{qjv}N_{pv}) \\
B_i = \;& L_1^2(\tfrac{4}{3}N_{pq}N_{pi,q} - \tfrac{8}{15}N_{ip}N_{pq,q}) \\
& + 2e_{pir}N_{qr}(\hat{L}_2^2 e_{puv}N_{qv,u} + \hat{L}_3^2 e_{quv}N_{pv,u}) \\
C = \;& L_1^2(\tfrac{1}{3}N_{ij,k}(N_{ij,k} + 2N_{jk,i}) - \tfrac{4}{15}N_{ki,i}N_{kj,j}) \\
& + e_{pir}N_{qr,i}(\hat{L}_2^2 e_{puv}N_{qv,u} + \hat{L}_3^2 e_{quv}N_{pv,u}) \; ,
\end{aligned} \tag{A.9}$$

where $\hat{L}_2^2 = \frac{4}{3}L_2^2 + \frac{8}{5}L_3^2$, $\hat{L}_3^2 = \frac{4}{3}L_2^2 - \frac{8}{5}L_3^2$, and e_{ijk} is the alternating symbol. Derivations of these expressions can be found in [12, 27].

A.2 Proof of the minimum principle

Following the treatment in [14], definitions

$$\bar{\mathbf{A}} = \begin{bmatrix} A_{11} & A_{12} & A_{13} & \frac{1}{2}B_1 \\ A_{21} & A_{22} & A_{23} & \frac{1}{2}B_2 \\ A_{31} & A_{32} & A_{33} & \frac{1}{2}B_3 \\ \frac{1}{2}B_1 & \frac{1}{2}B_2 & \frac{1}{2}B_3 & 1+C \end{bmatrix} \tag{A.10}$$

and

$$\mathbf{e} = \left[\dot{\epsilon}^p_{,1},\; \dot{\epsilon}^p_{,2},\; \dot{\epsilon}^p_{,3},\; \dot{\epsilon}^p\right]^T \tag{A.11}$$

are introduced to simplify the derivation. With these definitions, the generalized plastic strain rate $\dot{\Lambda}^p$ can be rewritten as

$$(\dot{\Lambda}^p)^2 = \bar{A}_{ij} e_i e_j \ .$$

The following lemma will be used in the proof of the minimum principle.

Lemma 1. The matrix $\bar{\mathbf{A}}$ defined in (A.10) is symmetric and strictly positive definite if the flow direction $\mathbf{N}$ does not degenerate ($N_{ij}N_{ij} = \frac{3}{2}$ holds).

Proof. The symmetry of $\bar{\mathbf{A}}$ is obvious based on the expression (A.10).

For any $\mathbf{e} \in \mathbb{R}^4$, we can define

$$\rho_{ijk} = e_k N_{ij} + e_4 N_{ij,k} \ . \tag{A.12}$$

Because $\rho_{ijk} = \rho_{jik}$ and $\rho_{iik} = 0$, there is a unique orthogonal decomposition ([12, 27])

$$\rho_{ijk} = \rho^{(1)}_{ijk} + \rho^{(2)}_{ijk} + \rho^{(3)}_{ijk} \ .$$

As a result, we can rewrite $\bar{A}_{ij} e_i e_j$ as follows:

$$\bar{A}_{ij} e_i e_j = (e_4)^2 + \sum_{i,j=1}^{3} A_{ij} e_i e_j + \sum_{i=1}^{3} B_i e_i e_4 + C (e_4)^2 \tag{A.13}$$

$$= (e_4)^2 + L_1^2 \rho^{(1)}_{ijk} \rho^{(1)}_{ijk} + 4 L_2^2 \rho^{(2)}_{ijk} \rho^{(2)}_{ijk} + \frac{8}{3} L_3^2 \rho^{(3)}_{ijk} \rho^{(3)}_{ijk} \ , \tag{A.14}$$

which implies

$$\bar{A}_{ij} e_i e_j \geq 0$$

for any $\mathbf{e}$, and $\bar{\mathbf{A}}$ is positive definite.

When $\bar{A}_{ij} e_i e_j = 0$, Eq (A.14) implies $e_4 = 0$ and $\rho^{(m)}_{ijk} = 0$ for all $i, j, k, m \in \{1, 2, 3\}$, which yields

$$\rho_{ijk} = \rho^{(1)}_{ijk} + \rho^{(2)}_{ijk} + \rho^{(3)}_{ijk} = 0 \ .$$

Because of the definition in Eq (A.12), we have $e_k N_{ij} = 0$ for all $i, j, k \in \{1, 2, 3\}$.

Using the condition $N_{ij}N_{ij} = \frac{3}{2}$, we can get

$$0 = (e_k)^2 N_{ij}N_{ij} = \frac{3}{2}(e_k)^2 \ ,$$

from which $e_k = 0$ for $k \in \{1,2,3\}$ is obtained immediately. In sum, $\mathbf{e} = 0$ when $\bar{A}_{ij}e_ie_j = 0$. □

The minimum principle in the strain gradient model of Fleck and Hutchinson is stated in the following theorem:

Theorem 1. Assume that a solid body occupies a domain $V \in \mathbb{R}^3$ with boundary $S = S_T \cup S_U$. Traction rates $\dot{\mathbf{t}}$ and $\dot{\tau}$ are applied on S_T. Velocity and effective plastic strain rate $\{\dot{\mathbf{u}}, \dot{\epsilon}^p\}$ are prescribed on S_U with $|S_U| > 0$. Then the exact rates $\{\dot{\mathbf{u}}^*, \dot{\epsilon}^{p*}\}$ are a unique minimum of the functional

$$I(\dot{\mathbf{u}}, \dot{\epsilon}^p) = \frac{1}{2}\int_V C_{ijkl}(\dot{E}_{ij} - \dot{\epsilon}^p N_{ij})(\dot{E}_{kl} - \dot{\epsilon}^p N_{kl}) + h(\Lambda^p)(\dot{\Lambda}^p)^2 \, dV - \int_{S_T} \dot{t}_i\dot{u}_i + \dot{\tau}\dot{\epsilon}^p \, dS \ ,$$

on the set $\mathscr{Y}$, which is defined by

$$\mathscr{Y} = \left\{\{\dot{\mathbf{u}}, \dot{\epsilon}^p\} \in H^1(V,\mathbb{R}^3) \times H^1(V,\mathbb{R}) \middle| \ \dot{\mathbf{u}} = \dot{\mathbf{u}}^0 \text{ and } \dot{\epsilon}^p = \dot{\epsilon}^{p0} \text{ on } S_U, \ \dot{\epsilon}^p \geq 0, \ \dot{\epsilon}^p(\Sigma - \Sigma^Y) = 0\right\} \ .$$

Proof. Assume $\{\dot{\mathbf{u}}^*, \dot{\epsilon}^{p*}\} \in \mathscr{Y}$ are the exact rates. For any variable $(\bullet)$ and the variable with star $(\bullet)^*$, denote the difference operater as $\Delta(\bullet) = (\bullet) - (\bullet)^*$.

The functions

$$V^e(\mathbf{W}) = \frac{1}{2}C_{ijkl}W_{ij}W_{kl} \quad \text{and} \quad V^p(\xi) = \frac{1}{2}h\xi^2$$

are convex and smooth with respect to their own variables. Therefore the following inequalities for the convex functions hold:

$$\Delta V^e \geq \frac{\partial V^e}{\partial W_{ij}}|_{\mathbf{W}^*_{ij}} \Delta W \;, \tag{A.15}$$

$$\Delta V^p \geq \frac{\partial V^p}{\partial \xi}|_{\xi^*} \Delta \xi \;. \tag{A.16}$$

The difference between the value of the functional at an arbitrary $(\dot{\mathbf{u}}, \dot{\epsilon}^p) \in \mathscr{Y}$ and the value of the functional at $\{\dot{\mathbf{u}}^*, \dot{\epsilon}^{p*}\}$ can be written as follows:

$$\begin{aligned}
&I(\dot{\mathbf{u}}, \dot{\epsilon}^p) - I(\dot{\mathbf{u}}^*, \dot{\epsilon}^{p*}) \\
&= \int_V V^e(\dot{\mathbf{E}}^e) - V^e(\dot{\mathbf{E}}^{e*}) + V^p(\dot{\Lambda}^p) - V^p(\dot{\Lambda}^{p*}) \, dV - \int_{S_T} \dot{t}_i \Delta \dot{u}_i + \dot{\tau} \Delta \dot{\epsilon}^p \, dS \\
&\geq \int_V C_{ijkl} \dot{E}^{e*}_{kl} \Delta \dot{E}^e_{ij} + h \dot{\Lambda}^{p*} \Delta \dot{\Lambda}^p \, dV - \int_{S_T} \dot{t}_i \Delta \dot{u}_i + \dot{\tau} \Delta \dot{\epsilon}^p \, dS \\
&= \int_V T^*_{ij} (\Delta \dot{E}_{ij} - \Delta \dot{E}^p_{ij}) + h \dot{\Lambda}^{p*} \Delta \dot{\Lambda}^p \, dV - \int_S \dot{t}_i \Delta \dot{u}_i + \dot{\tau} \Delta \dot{\epsilon}^p \, dS \quad (\dot{T}^*_{ij} n_j = \dot{t}_i, \; \dot{m}^*_i n_i = \dot{\tau}) \\
&= \int_V \dot{T}^*_{ij} (\Delta \dot{E}_{ij} - \Delta \dot{E}^p_{ij}) + h \dot{\Lambda}^{p*} \Delta \dot{\Lambda}^p \, dV - \int_S \dot{T}^*_{ij} n_j \Delta \dot{u}_i + \dot{m}^*_i n_i \Delta \dot{\epsilon}^p \, dS \\
&= \int_V \dot{T}^*_{ij} (\Delta \dot{E}_{ij} - \Delta \dot{E}^p_{ij}) + h \dot{\Lambda}^{p*} \Delta \dot{\Lambda}^p \, dV - \int_V \dot{T}^*_{ij,j} \Delta \dot{u}_i + \dot{T}^*_{ij} \Delta \dot{E}_{ij} + \dot{m}^*_{i,i} \Delta \dot{\epsilon}^p + \dot{m}^*_i \Delta \dot{\epsilon}^p_{,i} \, dV \\
&= \int_V -\dot{T}^*_{ij} \Delta \dot{E}^p_{ij} + h \dot{\Lambda}^{p*} \Delta \dot{\Lambda}^p - \dot{m}^*_{i,i} \Delta \dot{\epsilon}^p - \dot{m}^*_i \Delta \dot{\epsilon}^p_{,i} \, dV \quad (\dot{T}^*_{ij,j} = 0) \\
&= \int_V (-\dot{\sigma}^{ef*} - \dot{m}^*_{i,i}) \Delta \dot{\epsilon}^p + h \dot{\Lambda}^{p*} \Delta \dot{\Lambda}^p - \dot{m}^*_i \Delta \dot{\epsilon}^p_{,i} \, dV \quad (\dot{T}^*_{ij} \Delta \dot{E}^p_{ij} = \dot{\sigma}^{ef*} \Delta \dot{\epsilon}^p) \\
&= \int_V -\dot{\Sigma}^* \Delta \dot{\epsilon}^p - \dot{m}^*_i \Delta \dot{\epsilon}^p_{,i} + h \dot{\Lambda}^{p*} \Delta \dot{\Lambda}^p \, dV \;. \quad (\dot{\Sigma}^* = \dot{\sigma}^{ef*} + \dot{m}^*_{i,i})
\end{aligned} \tag{A.17}$$

First of all, for simplicity, assume $\dot{\epsilon}^{p*} > 0$ holds throughout the domain. Then

$$\dot{\Sigma}^* = \dot{\Sigma}^Y = h[(1 + C) \dot{\epsilon}^{p*} + \frac{1}{2} B_i \dot{\epsilon}^{p*}_{,i}] \;.$$

As a result, we can obtain

$$
\begin{aligned}
&\dot{\Sigma}^* \dot{\epsilon}^p + \dot{m}_i^* \dot{\epsilon}^p_{,i} \\
&= \dot{\Sigma}^Y \dot{\epsilon}^p + \dot{m}_i^* \dot{\epsilon}^p_{,i} \\
&= h[(1+C)\dot{\epsilon}^{p*} + \frac{1}{2} B_i \dot{\epsilon}^{p*}_{,i}]\dot{\epsilon}^p + h[A_{ij}\dot{\epsilon}^{p*}_{,j} + \frac{1}{2} B_i \dot{\epsilon}^{p*}]\dot{\epsilon}^p_{,i} \\
&= h[(1+C)\dot{\epsilon}^{p*}\dot{\epsilon}^p + \frac{1}{2} B_i (\dot{\epsilon}^{p*}\dot{\epsilon}^p_{,i} + \dot{\epsilon}^p \dot{\epsilon}^{p*}_{,i}) + A_{ij}\dot{\epsilon}^{p*}_{,j}\dot{\epsilon}^p_{,i}] \\
&= h\bar{A}_{ij} e_i^* e_j \ ,
\end{aligned}
\tag{A.18}
$$

and also the identity

$$
\dot{\Sigma}^* \dot{\epsilon}^{p*} + \dot{m}_i^* \dot{\epsilon}^{p*}_{,i} = h\bar{A}_{ij} e_i^* e_j^* = h(\dot{\Lambda}^{p*})^2 \ ,
$$

which is a special case of Eq (A.18). Now, continue the proof from the inequality (A.17).

$$
\begin{aligned}
&I(\dot{\mathbf{u}}, \dot{\epsilon}^p) - I(\dot{\mathbf{u}}^*, \dot{\epsilon}^{p*}) \\
&\geq \int_V h\dot{\Lambda}^{p*}(\dot{\Lambda}^p - \dot{\Lambda}^{p*}) - \dot{\Sigma}^*(\dot{\epsilon}^p - \dot{\epsilon}^{p*}) - \dot{m}_i^*(\dot{\epsilon}^p_{,i} - \dot{\epsilon}^{p*}_{,i}) \, dV \\
&= \int_V h\dot{\Lambda}^{p*}\dot{\Lambda}^p - \dot{\Sigma}^*\dot{\epsilon}^p - \dot{m}_i^*\dot{\epsilon}^p_{,i} - h(\dot{\Lambda}^{p*})^2 + \dot{\Sigma}^*\dot{\epsilon}^{p*} + \dot{m}_i^*\dot{\epsilon}^{p*}_{,i} \, dV \\
&= \int_V h\dot{\Lambda}^{p*}\dot{\Lambda}^p - \dot{\Sigma}^*\dot{\epsilon}^p - \dot{m}_i^*\dot{\epsilon}^p_{,i} \, dV \\
&= \int_V h(\bar{A}_{ij} e_i^* e_j^*)^{\frac{1}{2}} (\bar{A}_{kl} e_k e_l)^{\frac{1}{2}} - h\bar{A}_{ij} e_i^* e_j \, dV \\
&= \int_V h[(\bar{A}_{ij} e_i^* e_j^*)^{\frac{1}{2}} (\bar{A}_{kl} e_k e_l)^{\frac{1}{2}} - \bar{A}_{ij} e_i^* e_j] \, dV \\
&\geq 0
\end{aligned}
\tag{A.19}
$$

In the last inequality of Eq (A.19), Cauchy inequality has been used in the following way:

$$\begin{aligned}
\bar{A}_{ij}e_i^*e_j &= (\mathbf{e}^*)^T\bar{\mathbf{A}}\mathbf{e} \\
&= (\mathbf{e}^*)^T\bar{\mathbf{A}}^{\frac{1}{2}}\bar{\mathbf{A}}^{\frac{1}{2}}\mathbf{e} \\
&= (\bar{\mathbf{A}}^{\frac{1}{2}}\mathbf{e}^*)^T(\bar{\mathbf{A}}^{\frac{1}{2}}\mathbf{e}) \\
&\leq \|\bar{\mathbf{A}}^{\frac{1}{2}}\mathbf{e}^*)\|_2\|\bar{\mathbf{A}}^{\frac{1}{2}}\mathbf{e}\|_2 \\
&= (\bar{A}_{ij}e_i^*e_j^*)^{\frac{1}{2}}(\bar{A}_{kl}e_ke_l)^{\frac{1}{2}}
\end{aligned} \tag{A.20}$$

where $\bar{\mathbf{A}}$ is symmetric and strictly positive definite upon plastic loading (Lemma 1). Up to now, the proof is achieved for the case that plastic loading occurs throughout the domain. For a general situation, the proof follows from the decomposition of the domain V:

$$V = \{x \in V |\ \dot{\epsilon}^{p*} > 0\} \cup \{x \in V |\ \dot{\epsilon}^{p*} = 0\}\ .$$

Starting from the inequality (A.17),

$$\begin{aligned}
I(\dot{\mathbf{u}}, \dot{\epsilon}^p) - I(\dot{\mathbf{u}}^*, \dot{\epsilon}^{p*}) &\geq \int_V -\dot{\Sigma}^*\Delta\dot{\epsilon}^p - \dot{m}_i^*\Delta\dot{\epsilon}^p_{,i} + h\dot{\Lambda}^{p*}\Delta\dot{\Lambda}^p\, dV \\
&= \int_{\{x\in V|\ \dot{\epsilon}^{p*}>0\}} -\dot{\Sigma}^*\Delta\dot{\epsilon}^p - \dot{m}_i^*\Delta\dot{\epsilon}^p_{,i} + h\dot{\Lambda}^{p*}\Delta\dot{\Lambda}^p\, dV \\
&+ \int_{\{x\in V|\ \dot{\epsilon}^{p*}=0\}} -\dot{\Sigma}^*\Delta\dot{\epsilon}^p - \dot{m}_i^*\Delta\dot{\epsilon}^p_{,i} + h\dot{\Lambda}^{p*}\Delta\dot{\Lambda}^p\, dV \\
&\geq \int_{\{x\in V|\ \dot{\epsilon}^{p*}=0\}} -\dot{\Sigma}^*\Delta\dot{\epsilon}^p - \dot{m}_i^*\Delta\dot{\epsilon}^p_{,i} + h\dot{\Lambda}^{p*}\Delta\dot{\Lambda}^p\, dV \\
&= \int_{\{x\in V|\ \dot{\epsilon}^{p*}=0\}} -\dot{\Sigma}^*\dot{\epsilon}^p\, dV \quad (\dot{\mathbf{m}}^* = 0,\ \dot{\Lambda}^{p*} = 0) \\
&\geq 0\ .
\end{aligned}$$

The last inequality holds because $\dot{\epsilon}^{p*} = 0$ implies $\dot{\Sigma}^* \leq 0$ or the current generalized effective stress Σ is strictly less than the current generalized yield stress Σ^Y. When $\dot{\Sigma}^* \leq 0$, the integrand $-\dot{\Sigma}^*\dot{\epsilon}^p$ is nonnegative. When the current generalized effective stress Σ is strictly less than Σ^Y, the stress state is not on the yield surface, which implies $\dot{\epsilon}^p = 0$ and the integrand is also zero. Therefore, no matter which case occurs, the integrand $-\dot{\Sigma}^*\dot{\epsilon}^p$ is always nonnegative.

In sum, the exact rates $\{\dot{\mathbf{u}}^*, \dot{\epsilon}^{p*}\}$ are a global minimum. Conditions for the convexity inequalities (A.15, A.16) and Cauchy inequality (A.20) to become equalities are

$$\dot{\mathbf{E}}^e = \dot{\mathbf{E}}^{e*} \quad \text{and} \quad \dot{\Lambda}^p = \dot{\Lambda}^{p*} ,$$

which suggest that for any $\{\dot{\mathbf{u}}, \dot{\epsilon}^p\} \in \mathscr{Y}$ satisfying $\Delta I = 0$, the equalities $\dot{\epsilon}^p = \dot{\epsilon}^{p*}$ and $\dot{\mathbf{E}} = \dot{\mathbf{E}}^*$ must hold in the domain. Since only the isotropic material is considered here, the elasticity tensor has the expression

$$C_{ijkl} = \lambda\delta_{ij}\delta_{kl} + \mu(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk})$$

with Láme constants $\lambda > 0$ and $\mu > 0$. This guarantees that the H^1 norm of the displacement and the energy norm of the strain induced by the displacement are equivalent on $H_0^1(V)$ (Page 274 in [20]). As a result, $\dot{\mathbf{E}} = \dot{\mathbf{E}}^*$ in V together with $|S_U| > 0$ yields

$$\dot{\mathbf{u}} = \dot{\mathbf{u}}^* \quad \text{a.e. in } V .$$

Finally, the proof of the uniqueness of the minimum is complete.

□

A.3 Derivation of the optimality conditions

In this section, the optimality conditions associated with the functional (2.14) in the Fleck and Hutchinson's model are derived based on a general expression of the generalized effective plastic strain rate.

The general expression of the generalized effective plastic strain rate reads

$$\dot{\Lambda}^p = \left\{(\dot{\epsilon}^p)^\mu + [A_{ij}\dot{\epsilon}^p_{,i}\dot{\epsilon}^p_{,j} + B_i\dot{\epsilon}^p_{,i}\dot{\epsilon}^p + C(\dot{\epsilon}^p)^2]^{\frac{\mu}{2}}\right\}^{\frac{1}{\mu}} \quad \text{for } 1 \le \mu \le 2 . \tag{A.21}$$

Assume $\{\dot{\mathbf{u}}, \dot{\epsilon}^p\}$ is a stationary point of the functional (2.14) with the generalized effective plastic strain rate defined in Eq (A.21); then the first order variation of the functional should be zero.

The variation with respect to $\dot{\mathbf{u}}$ reads

$$
\begin{aligned}
0 &= \lim_{t\to 0} \frac{I(\dot{u}_i + t\delta\dot{u}_i, \dot{\epsilon}^p) - I(\dot{u}_i, \dot{\epsilon}^p)}{t} \qquad \forall\ \delta\dot{u}_i \text{ s.t. } \delta\dot{u}_i = 0 \text{ on } S_U \\
&= \int_V C_{ijkl}(\dot{E}_{ij} - \dot{\epsilon}^p N_{ij})\delta\dot{E}_{ij}\, dV - \int_{S_T} \dot{t}_i \delta\dot{u}_i\, dS \\
&= \int_V C_{ijkl}(\dot{E}_{ij} - \dot{\epsilon}^p N_{ij})\delta\dot{E}_{ij}\, dV - \int_S \dot{t}_i \delta\dot{u}_i\, dS \\
&= \int_V \dot{T}_{ij}\delta\dot{E}_{ij}\, dV - \int_S \dot{t}_i \delta\dot{u}_i\, dS \\
&= \int_V -\dot{T}_{ij,j}\delta\dot{u}_i\, dV + \int_S \dot{T}_{ij}n_j\delta\dot{u}_i\, dS - \int_S \dot{t}_i\delta\dot{u}_i\, dS \\
&= \int_V -\dot{T}_{ij,j}\delta\dot{u}_i\, dV + \int_S (\dot{T}_{ij}n_j - \dot{t}_i)\delta\dot{u}_i\, dS\ .
\end{aligned}
$$

Since $\delta\dot{u}_i$ is arbitrary, the variational equation above yields the conventional equilibrium equations

$$\dot{T}_{ij,j} = 0 \quad \text{in } V \quad \text{and} \quad \dot{T}_{ij}n_j = \dot{t}_i \text{ on } S_T\ . \tag{A.22}$$

In order to simplify the notations, a 4 by 4 matrix

$$\hat{\mathbf{A}} = \begin{bmatrix} A_{11} & A_{12} & A_{13} & \frac{1}{2}B_1 \\ A_{21} & A_{22} & A_{23} & \frac{1}{2}B_2 \\ A_{31} & A_{32} & A_{33} & \frac{1}{2}B_3 \\ \frac{1}{2}B_1 & \frac{1}{2}B_2 & \frac{1}{2}B_3 & C \end{bmatrix} \tag{A.23}$$

and a vector $\mathbf{e} = \left[\dot{\epsilon}^p_{,1},\ \dot{\epsilon}^p_{,2},\ \dot{\epsilon}^p_{,3},\ \dot{\epsilon}^p\right]^T$ are introduced to derive the variational results with respect to $\dot{\epsilon}^p$. With these definitions, the contribution of the plastic strain gradients in the generalized effective plastic strain rates can be simplified as

$$A_{ij}\dot{\epsilon}^p_{,i}\dot{\epsilon}^p_{,j} + B_i\dot{\epsilon}^p_{,i}\dot{\epsilon}^p + C(\dot{\epsilon}^p)^2 = \hat{A}_{ij}e_ie_j\ .$$

Define the set of the material points that undergo plastic loading by

$$V^p = \{x \in V |\ \dot{\epsilon}^p > 0\}\ ,$$

and then the set for admissible $\delta\dot{\epsilon}^p$ can be specified by

$$\mathscr{X} = \{\delta\dot{\epsilon}^p |\ \delta\dot{\epsilon}^p = 0 \text{ if } x \in V \setminus V^p \text{ or } x \in\ S_U\}\ .$$

The variation with respect to $\dot{\epsilon}^p$ reads

$$\begin{aligned}
0 &= \lim_{t \to 0} \frac{I(\dot{\mathbf{u}}, \dot{\epsilon}_p + t\delta\dot{\epsilon}^p) - I(\dot{\mathbf{u}}, \dot{\epsilon}^p)}{t} \qquad \forall\ \delta\dot{\epsilon}^p \in \mathscr{X} \\
&= \int_{V^p} \frac{h}{2} \delta(\dot{\Lambda}^p)^2\, dV - \int_{S_T} \dot{\tau}\delta\dot{\epsilon}^p\, dS - \int_{V^p} \dot{T}_{kl} N_{kl} \delta\dot{\epsilon}^p\, dV \\
&= \int_{V^p} \frac{h}{\mu} [(\dot{\epsilon}^p)^\mu + (\hat{A}_{ij} e_i e_j)^{\frac{\mu}{2}}]^{\frac{2}{\mu}-1} \delta[(\dot{\epsilon}^p)^\mu + (\hat{A}_{ij} e_i e_j)^{\frac{\mu}{2}}]\, dV - \int_{S_T} \dot{\tau}\delta\dot{\epsilon}^p\, dS - \int_{V^p} \dot{\sigma}^{ef} \delta\dot{\epsilon}^p\, dV \\
&= \int_{V^p} \frac{h}{\mu} [(\dot{\epsilon}^p)^\mu + (\hat{A}_{ij} e_i e_j)^{\frac{\mu}{2}}]^{\frac{2}{\mu}-1} [\mu(\dot{\epsilon}^p)^{\mu-1}\delta\dot{\epsilon}^p + \frac{\mu}{2}(\hat{A}_{ij} e_i e_j)^{\frac{\mu}{2}-1} 2\hat{A}_{kl} e_k \delta e_l]\, dV \\
&\quad - \int_{S_T} \dot{\tau}\delta\dot{\epsilon}^p\, dS - \int_{V^p} \dot{\sigma}^{ef} \delta\dot{\epsilon}^p\, dV \\
&= \int_{V^p} h[(\dot{\epsilon}^p)^\mu + (\hat{A}_{ij} e_i e_j)^{\frac{\mu}{2}}]^{\frac{2}{\mu}-1} [(\dot{\epsilon}^p)^{\mu-1}\delta\dot{\epsilon}^p + (\hat{A}_{ij} e_i e_j)^{\frac{\mu}{2}-1} \hat{A}_{kl} e_k \delta e_l]\, dV \\
&\quad - \int_{S_T} \dot{\tau}\delta\dot{\epsilon}^p\, dS - \int_{V^p} \dot{\sigma}^{ef} \delta\dot{\epsilon}^p\, dV \\
&= \int_{V^p} \underbrace{h[(\dot{\epsilon}^p)^\mu + (\hat{A}_{ij} e_i e_j)^{\frac{\mu}{2}}]^{\frac{2}{\mu}-1} [(\dot{\epsilon}^p)^{\mu-1} + (\hat{A}_{ij} e_i e_j)^{\frac{\mu}{2}-1} (\frac{B_k}{2}\dot{\epsilon}^p_{,k} + C\dot{\epsilon}^p)]}_{\alpha}\, \delta\dot{\epsilon}^p\, dV \\
&\quad + \int_{V^p} \underbrace{h[(\dot{\epsilon}^p)^\mu + (\hat{A}_{ij} e_i e_j)^{\frac{\mu}{2}}]^{\frac{2}{\mu}-1} [(\hat{A}_{ij} e_i e_j)^{\frac{\mu}{2}-1} (A_{kl}\dot{\epsilon}^p_{,k} + \frac{B_l}{2}\dot{\epsilon}^p)]}_{\beta_l}\, \delta\dot{\epsilon}^p_{,l}\, dV \\
&\quad - \int_{S_T} \dot{\tau}\delta\dot{\epsilon}^p\, dS - \int_{V^p} \dot{\sigma}^{ef} \delta\dot{\epsilon}^p\, dV \\
&= \int_{V^p} (\alpha - \beta_{l,l} - \dot{\sigma}^{ef}) \delta\dot{\epsilon}^p\, dV - \int_{S_T} \dot{\tau}\delta\dot{\epsilon}^p\, dS + \int_{\partial V^p} \beta_l n_l \delta\dot{\epsilon}^p\, dS
\end{aligned} \tag{A.24}$$

Divergence theorem is applied to eliminate $\delta\dot{\epsilon}^p_{,l}$ from the volumetric integration in the last equation. The set ∂V^p represents the surface of the domain V^p, which can be partitioned as follows:

$$\partial V^p = (\partial V^p \cap V) \cup (\partial V^p \cap S_U) \cup (\partial V^p \cap S_T)\,. \tag{A.25}$$

For $x \in (\partial V^p \cap V) \cup (\partial V^p \cap S_U)$, we have $\delta\epsilon^p = 0$. Also it is reasonable to assert that $\partial V^p \cap S_T = S_T$, since the higher order traction τ is only associated with the plastic loading. With these considerations, Eq (A.24) can be written as

$$\begin{aligned} 0 &= \int\limits_{V^p} (\alpha - \beta_{l,l} - \dot{\sigma}^{ef})\delta\dot{\epsilon}^p \, dV - \int\limits_{S_T} \dot{\tau}\delta\dot{\epsilon}^p \, dS + \int\limits_{\partial V^p} \beta_l n_l \delta\dot{\epsilon}^p \, dS \\ &= \int\limits_{V^p} (\alpha - \beta_{l,l} - \dot{\sigma}^{ef})\delta\dot{\epsilon}^p \, dV + \int\limits_{S_T} (\beta_l n_l - \dot{\tau})\delta\dot{\epsilon}^p \, dS \end{aligned} \tag{A.26}$$

Since $\delta\epsilon^p$ is arbitrary, the variational equation above yields the non-conventional equilibrium equations

$$\alpha - \beta_{l,l} - \dot{\sigma}^{ef} = 0 \quad \text{in } V^p \quad \text{and} \quad \beta_l n_l = \dot{\tau} \quad \text{on } S_T\,. \tag{A.27}$$

This is as far as the variation can take us. In the next section, we will introduce some definitions to explain these variational results.

Comments

Regarding the results derived from the Principle of Virtual Work (Eq (2.10))

$$\Sigma = m_{i,i} + \sigma^{ef} \text{ in } V \quad \text{and} \quad m_i n_i = \tau \text{ on } S_T$$

and also the structure of the variational results (A.27), it is natural to define the rate of the generalized yield stress and the rate of the higher order stresses by the following expressions:

$$\dot{\Sigma}^Y = \alpha = h[(\dot{\epsilon}^p)^\mu + (\hat{A}_{ij}e_ie_j)^{\frac{\mu}{2}}]^{\frac{2}{\mu}-1}[(\dot{\epsilon}^p)^{\mu-1} + (\hat{A}_{ij}e_ie_j)^{\frac{\mu}{2}-1}(\frac{B_k}{2}\dot{\epsilon}^p_{,k} + C\dot{\epsilon}^p)] \ , \quad \text{(A.28)}$$

$$\dot{m}_l = \beta_l = h[(\dot{\epsilon}^p)^\mu + (\hat{A}_{ij}e_ie_j)^{\frac{\mu}{2}}]^{\frac{2}{\mu}-1}[(\hat{A}_{ij}e_ie_j)^{\frac{\mu}{2}-1}(A_{kl}\dot{\epsilon}^p_{,k} + \frac{B_l}{2}\dot{\epsilon}^p)], \quad l = 1, 2, 3 \ . \quad \text{(A.29)}$$

With these definitions, the variational results (A.27) can be reformulated as follows:

$$\dot{\Sigma} = \dot{\Sigma}^Y = \dot{m}_{l,l} + \dot{\sigma}^{ef} \quad \text{in } V^p \ , \quad \text{(A.30)}$$

$$\dot{m}_l n_l = \dot{\tau} \qquad \text{on } S_T \ . \quad \text{(A.31)}$$

Eq (A.30) describes the yield condition upon plastic loading, while Eq (A.31) describes the rate form of the higher order traction boundary condition.

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