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Nonlocal gradient-dependent modeling of plasticity with anisotropic hardening

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NONLOCAL GRADIENT-DEPENDENT MODELING OF PLASTICITY WITH ANISOTROPIC HARDENING

A Thesis

Submitted to the Graduate Faculty of the Louisiana State University and Agricultural and Mechanical College in partial fulfillment of the requirements for the degree of Master of Science In Civil Engineering in The Department of Civil Engineering

by
Gerald Pekmezi
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ABSTRACT

This work is concerned with the formulation of the thermodynamics of nonlocal plasticity using the gradient theory. The formulation is based on the nonlocality energy residual introduced by Eringen and Edelen (1972). Gradients are introduced for those variables associated with isotropic and kinematic hardening. The formulation applies to small strain gradient plasticity and makes use of the evanescent memory model for kinematic hardening. This is accomplished using the kinematic flux evolution as developed by Zbib and Aifantis (1987). Therefore, the present theory is a four nonlocal parameter-based theory that accounts for the influence of large variations in the plastic strain, accumulated plastic strain, accumulated plastic strain gradients, and the micromechanical evolution of the kinematic flux. Using the principle of virtual power and the laws of thermodynamics, thermodynamically-consistent equations are derived for the nonlocal plastic yield criterion and associated flow rule. The presence of higher-order gradients in the plastic strain is shown to enhance a corresponding history variable which arises from the accumulation of the plastic strain gradients. Furthermore, anisotropy is introduced by plastic strain gradients in the form of kinematic hardening. Plastic strain gradients can be attributed to the net Burgers vector, while gradients in the accumulation of plastic strain are responsible for the introduction of isotropic hardening. The equilibrium between internal Cauchy stress and the microstresses conjugate to the higher-order gradients frames the yield criterion, which is obtained from the principle of virtual power. Microscopic boundary conditions, associated with plastic flow, are introduced to supplement the macroscopic boundary conditions of classical plasticity. The nonlocal formulation developed here preserves the classical assumption of local plasticity, wherein
plastic flow direction is governed by the deviatoric Cauchy stress. The theory is applied to the problems of thin films on both soft and hard substrates. Numerical solutions are presented for bi-axial tension and simple shear loading of thin films on substrates.
1 INTRODUCTION

In the 1850s, the introduction of the Bessemer process facilitated construction using a material that until then had been considered too expensive to produce and use en masse. That material was steel and its availability sparked a structural revolution, whereby grander and grander scale structures became feasible. Since then, material engineering has advanced at an ever increasing pace, and today we have reached the point where we can engineer materials at scales approaching the atomic scale. However, in solid mechanics, as in most other branches of physics, we have found that mathematical models conceived for the “visible” or macro scale, become increasingly insufficient as we approach the discrete microstructure of the material. The need has therefore become evident for new models to capture relevant effects in the behavior of the material. The complexity of such models is key to their adequacy in describing the material behavior. However, the complexity of the models must also be limited to what is necessary, since increased complexity leads to increased cost (e.g. computational cost). One approach, favored in the present model, is to maintain the general framework of the macro-scale model (continuum mechanics), but to embed into it micromechanical characteristics which enable the composite model to describe the observed micro-scale effects.

The particular problem this model aims to address, is the introduction at the continuum plasticity level of the so-called “size effect”. Experimental observations reveal that, in many cases, the size of the material specimen and grain size significantly impacts deformation and failure. For example, it has been observed that, in the bending of thin films, decreasing the thickness of the films produces a strengthening effect on the film material. Similarly, micro-torsion tests of thin wires exhibit increased strength for smaller
diameters of the wires. Other effects of a similar nature include increased strength of particle-reinforced composites for decreased particle size, and increased hardness for smaller indentation size in micro-indentation tests. These effects are not compatible with the classical approach of continuum plasticity, where the material behavior is assumed to be the same even if its size is reduced ad infinitum. It seems, therefore, necessary to formulate a “coarse” model, one that has an embedded length scale to identify that scale where discrete events that occur in the microstructure are relevant to the material behavior in the physical scale.

The aforementioned problem has been tackled by a number of researchers using a range of models, which can be collectively placed under the umbrella of nonlocal models. A nonlocal model is one where the evolution of a state variable (or tensor) at a particular point in the material, is dependent not only on the internal state of the point itself, but also on the state of the neighboring points. In general, this influence is weighed spatially, whereby the magnitude of the influence of a neighboring point is related to the proximity of the point. Examples of micro, meso and macro models that deal with the size effect in plasticity include molecular dynamics, discrete dislocation dynamics, and higher-order extension of classical plasticity. The first two types involve completely different physics than those used in local (classical) plasticity; atoms/molecules/dislocations are modeled individually and their interactions simulated. This means that the models are incapable of modeling materials in physical scales, as the computational effort necessary is beyond what is available.

By contrast, higher-order models such as the gradient model, maintain the framework of continuum mechanics, but introduce effects from higher order derivatives
or integrals of constitutive variables. A model that contains higher-order variables is inherently nonlocal, since its constitutive equations result in having one point in the continuum influence the other. The realization of higher-order modeling is varied. The formulation strategy can be to either heuristically introduce higher-order dependence directly into the constitutive equations, or to derive the constitutive equations by means of suitable energy arguments. The second strategy involves higher-order stresses in addition to higher-order strains, which means that additional boundary conditions are required. The first strategy is easier to implement, since it does not involve higher-order stresses. The means by which the higher order strains are introduced is either through integral-type models, explicit gradient models, or implicit gradient models which are in essence equivalent to integral-type models. The explicit gradient models are essentially weak forms of the integral-type models and are most suitable for implementation in numerical computations.

The formulation presented here is based on the nonlocality energy residual introduced by Eringen and Edelen (1972). The model applies to small strain gradient plasticity and makes use of the Armstrong-Frederick-type model for kinematic hardening proposed by Voyiadjis and Abu Al-Rub (2003).
2 Literature Review

A number of theoretical and numerical models have been proposed to overcome the lack of a length scale in the classical theory of plasticity. These include discrete dislocation dynamics simulations (Nicola et al., 2001, 2003), molecular dynamics simulations (Schiotz et al., 1998), crystal plasticity theories (Voyiadjis and Huang, 1996, Bittencourt et al., 2003), and strain gradient plasticity theories such as the one proposed here. These models have been termed “nonlocal models” (Nilsson, 1998, Stromberg and Ristinmaa, 1996).

The common thread in these models is that a nonlocal quantity is incorporated as the average of the corresponding local field quantity weighted spatially over an appropriate, finite volume surrounding the point under consideration. Oftentimes, this nonlocal quantity is resolved through the use of an integral format. In this format the associated intrinsic length scale influences the weight amplitude in proximity to a material point. Then there are plasticity formulations that make use of a gradient-enhanced model (De Borst and Muhlhaus, 1992). The benefit provided by these formulations, is that the integral format is avoided by approximating the nonlocal kernel with a Taylor series expansion. This yields a differential rather than integral, format.

The gradient formulation may be considered a higher-order extension of the local plasticity theory. The introduction of strain gradients into the local theory formulations leads to boundary value problems governed by partial differential equations of higher order with non-standard boundary conditions. There are essentially two strategies for the strain gradient theory formulations: one consists in heuristically introducing the gradient dependence directly into the constitutive equations of the local-type material. This
framework of strain gradient plasticity theories does not involve the higher-order stress, and requires no additional boundary conditions. The plastic strain gradient (or inverse elastic strain gradient) comes into play through the incremental plastic modulus. Examples in this class include the works by (Acharya, 2000, Acharya and Beaudoin, 2000, Acharya, et al., 2004, Dai and Parks, 1997)). In the aforementioned works, strain gradient hardening is assumed to be accounted for but not the work performed by the strain gradients in the material interior. It was concluded that the only possible formulation is a flow theory with strain gradient effects represented as an internal variable which acts to increase the current tangent hardening modulus. These theories are straightforward to implement in standard Finite Element (FE) codes. This particular approach was used in predicting polycrystal size effect and cleavage/orientation dependence in the fracture of ductile single crystals. However, criticism has been directed on the model’s capability due to the nonstandard boundary conditions (Niordson and Hutchinson, 2003, Volokh and Hutchinson, 2002) and the lack of systematic construction of the tangent modulus (Gao, et al., 1999).

In another class of strain gradient theory, formulations are derived by means of suitable energy arguments. A classical example of this strategy is the second strain gradient elasticity theory by Mindlin (1964) in which the higher order stresses are defined as the work conjugate of strain gradient by implying the virtual work principle and a strain energy potential incorporating the strain gradients. Along with the standard equilibrium equations, higher order nonlocal micro force balance equations are retrieved from the variational formulation of the virtual work principle. This additional equation requires the extra boundary conditions. Examples in this class include the works of Fleck
and Hutchinson (1997), Fleck and Hutchinson (2001) and Fleck, et al. (1994) where experimentally observed size effects have been modeled successfully. From a dimensional, consideration of an internal constitutive length parameter was introduced to scale the rotational gradient terms in the couple stress theory of the strain gradient plasticity. The physical basis of the length scale is connected to the storage of geometrically necessary dislocations (Ashby, 1970, Nye, 1953). They found in the twisting of thin copper wires that the scaled shear strength increases by a factor of three as the wire diameter decreases from 170 to 20 microns, while the increase of work hardening in simple tension is negligible.

Chen and Wang (2002) proposed the so-called new strain gradient theory, based on the general concept of couple stress theory. They implemented their new formulation to solve thin metallic wires in torsion and ultra thin metallic beam bending problems. It was concluded that if the boundary conditions are properly taken in their new theory, the results of the solution will predict the experimental findings provided by Fleck et al. (1994) and Stolken and Evans (1998). Xiang et al. (2006) used Fleck et al. (1994) strain gradient theory in order to capture the Bauschinger effect that is observed in the experimental investigations on Cu thin films with a passivation layer. From these experiments they found that thin films yield strength increased significantly with decreasing film thickness if one or both surfaces are passivated. By contrast, unpassivated thin films are relatively independent of film thickness and yield strength increases mainly as a result of grain size strengthening.

Gao et al. (1999), and Huang et al. (2000) proposed a Taylor based nonlocal theory of plasticity to account for the size dependency of the plastic deformation at the micron and
submicron scales. The length scale is related to the density of the geometrically necessary dislocations as introduced into the constitutive equations via the nonlocal variables which are expressed as an integral of local variables over all material points in the body. Gao and Huang (2001), Zhang et al. (2007), and Shi et al. (2008) applied this theory to micro-bending, micro tension, void growth, cavitations’ instabilities and particle reinforced composites. Their analyses results in identical predictions as in the mechanism-based strain gradient (MSG) plasticity. This higher order strain gradient theory is established from a multiscale, hierarchical framework to connect with the Taylor model in dislocation mechanics (Taylor, 1934, 1938). Results obtained using the MSG model agrees well with the work of McElhaney et al. (1998) on micro-indentation experiments of bulk copper, Gao et al. (1999) and Saha et al. (2001) on indentation experiments of aluminum thin film on a glass substrate, Fleck et al. (1994) on micro-torsion, Stolken and Evans (1998) on micro-bending experiments (see Gao, et al., 1999), and on metal-matrix composites (Xue, et al., 2002). It has also been successfully applied to study a few important problems at the micron and submicron scales, including microelectromechanical systems (Saha, et al., 2001), plastic flow localization (Shi, et al., 2000), and fracture (Jiang, 2001, Lu, et al., 2000).

Shi and Gao (2001) recently used the singular perturbation method to investigate a solid subjected to a constant body force, and showed that the effect of the higher-order stresses is significant only within a thin layer near the boundary of the material. Comparing the material length scale used in strain gradient theories, the thickness of the boundary layer is much smaller and is on the order of 10 nm., These results are interpreted by Huang et al. (2000) and Saha et al. (2001) as the higher-order stress has
little or essentially no effect on material properties that represent an average over the micron scale and above, such as the micro-indentation hardness. Therefore, they distinguished the effect of higher-order stress from the strain gradient effect by defining the former is within a thin boundary layer (thickness on the order of 10 nm) and the latter comes from the Taylor dislocation model and is important at the micron scale. As part of this separation they concluded that the effect of higher-order stress is negligible away from the thin boundary layer, and argued the possibility to develop a strain gradient plasticity theory based on the dislocation model to incorporate the strain gradient effects without the higher-order stress. The reason to eliminate the effect of higher order stress from the governing equations in such a theory is to avoid from the additional boundary conditions and to have essentially the same boundary conditions as in the conventional plasticity theories.

Gurtin (2004) developed a gradient theory of small deformation viscoplasticity based on the system of micro forces consistent with its peculiar balance, a mechanical version of the second law and a constitutive theory that includes Burgers vector through a free energy dependence on where represents the plastic part of the elastic plastic decomposition of the displacement gradient. Later Anand et al. (2005) studied the one dimensional theory of the strain gradient plasticity by performing analytical and numerical analyses by means of nonlocal finite element on three distinct physical phenomena such as internal variable hardening, energetic hardening with back stress associated with plastic strain gradient and dissipative strengthening associated with plastic strain rate and resulting in a size dependent increase in yield strength.
The Dislocation Dynamics (DD) and the molecular dynamics simulations are the alternative approaches to study small scale phenomena (Benzeraga and Shaver, 2006, Devincre, et al., 1997, Nicola, et al., 2003, Shu, et al., 2001, Zbib, et al., 2002). Shizawa and Zbib (1999) developed a thermodynamic theory of gradient elastoplasticity by introducing microstress which is conjugate to the dislocation density tensor. One of the drawbacks of these theories is that an additional set of parameters is required in order to specify the fundamental behavior of a single dislocation and the generation of new dislocations along with their interactions. Shen and Wang (2003) for 2D and Schiotz (2004) for 3D studied the influence of boundaries on dislocations from a continuum point of view. However, there are certain vital considerations that need to be addressed on the molecular dynamics simulations in the sense of the choice of the interatomic potential. The most commonly used potentials are empirical or semi-empirical. Furthermore there are limitations concerning dimensions as well as time. For instance, due to computational costs the simulations are limited to very short time intervals and high strain rates in order to reach interesting strain levels (Wolf et al., 2005, Lidorikis et al., 2001, Nakano et al., 2001).

Gudmundson (2004) formulated the small strain gradient plasticity for isotropic materials based on the balance law and dissipation inequality. He addressed boundary conditions and concluded that there is a close connection between surface energy of an interface and boundary conditions in terms of plastic strain and moment stress. A simple version of the theory was applied to a few examples such as biaxial loading of a thin film on thick substrate, torsion of thin wire and spherical void under remote hydrostatic tension in order to investigate the effect of varying length scales. This formulation is later
used to analyze the size dependent yield strength of thin films by Fredriksson and Gudmundson (2005). The results of their numerical analysis from these studies reveals that boundary layer is developed in the thin film for both biaxial and shear loading giving rise to size effects. These size effects are strongly connected to the buildup of surface energy at the interface. These effects of interface surface energy on the plastic deformation at the micron scale were motivated by Fredriksson and Gudmundson (2007) in order to conduct a detailed study on modeling of the interface between a thin film and a substrate. They addressed this issue within the framework of strain gradient plasticity and proposed two kinds of interface models for isotropic materials. First kind is based on the assumption that plastic work at the interface is completely stored as a surface energy and no dissipation occurred due to plasticity at the interface. In the second type it is assumed that the plastic work is completely dissipated and there is no build up of a surface energy. Two types of length scales are introduced one is for the behavior of the bulk material the other one is for the interface.

Their model can be considered in the same class of the existing interface models proposed by Cermelli and Gurtin (2002), Gurtin and Needleman (2005), Sun et al. (2000), Gurtin (2008), and Borg and Fleck (2007). Gurtin and Needleman (2005) and Cermelli and Gurtin (2002) addressed in their work the application of strain gradient plasticity for the case of crystal plasticity. In the case of Gurtin and Needleman (2005) they assumed continuity of the conjugate higher-order stresses on both sides of the interface. However, Cermelli and Gurtin (2002) assumed a jump at the interface of the conjugate higher order stresses. Both Gurtin and Needleman (2005) and Cermelli and Gurtin (2002) used dissipative mechanisms to model the interface (grain boundaries).
using a viscoplastic model that involved plastic slip rates at both sides of the interface as well as conjugate higher order stresses on both sides of the interface. In both cases they included discontinuities in plastic strains over the interface.

Willis and co-workers (Aifantis, et al., 2006, Aifantis and Willis, 2005, 2006) modeled the interface by a surface contribution to the strain energy that depends on the plastic strain at the interface. The distinct feature of this formulation is to introduce an interfacial yield stress that allows the interface to follow its own yield behavior. This interfacial yield stress is then described via dislocation transfer phenomena where its physical justification is made from observations of the nanoindentation near grain boundaries of body-centered cubic (bcc) metals. The main distinction of the work of Willis and co-workers from that of Gurtin and coworkers is that Willis and co-workers assumed a continuity in the plastic strain over the interface with a jump in the conjugate higher-order stresses.

Abu Al-Rub (2008) investigated the interfacial effect in parallel to the work of Willis and coworkers by using the higher order gradient dependent plasticity theory (Abu Al-Rub, et al., 2007, Voyiadjis and Abu Al-Rub, 2007) where microstress boundary conditions at the interface and free surfaces are enforced. In these works (Voyiadjis and Abu Al-Rub, 2007; Abu Al-Rub, 2008) they assumed that the total strain energy stored at the interface can be expressed in terms of the global nonlocality residual (Borino and Polizzotto, 1999, Borino and Polizzotto, 2003, Polizzotto, 2007, Polizzotto, et al., 2004).

Gudmundson (2004) presented a quite general discussion on the formulation of interface conditions within a strain gradient theory. He assumed discontinuity of both plastic strains and conjugate moment stresses over the interface. Fredriksson and
Gudmundson (2007) further discussed the distinctions among the above mentioned the interface models by presenting a mechanical analogy for the interface model.
As aforementioned, the impetus for the current research is provided by experimental results in the emerging areas of micro- and nanotechnology. These results exhibit distinct size dependence in the behavior of materials at the micron and submicron level. Specifically, strength differences have been observed to arise from continuous modification of the microstructural characteristics with changing size, whereby the smaller the size the higher the material strength appears to be.

In order to construct a mathematical formulation that properly models the observed effects, it is necessary to understand the behavior of the material at the most basic level that is relevant to plastic deformation. In this section, we review the physical mechanism by which plastic deformation occurs.

Physically, a dislocation is a crystallographic defect or irregularity in the crystal structure. Mathematically, the dislocation is a topological defect or a soliton. The mathematical description implies that dislocations behave as stable particles; they can move, grow and annihilate each other. At the microscopic level, plastic deformation in metallic materials is the end result of the collective behavior of a vast number of dislocations. Hence, crystallographic dislocation densities are appropriate metrics of plastic deformation in metals. These densities can be defined by their magnitude $\rho$ and are typically measured in line length per unit volume.

Plastic strain is directly related to the motion of dislocations. Meanwhile, hardening in metals is attributed to the interaction among dislocations and the interaction with the crystal microstructure nearby. These phenomena are driven by dislocation multiplication mechanisms: cross-slip and double cross-slip, glide, climb etc. Dislocations can also form
loops, aggregate at grain boundaries, and arrange themselves into varied types of substructures commonly called dislocation networks. These networks in turn constitute obstacles to the motion of other dislocations. This effect provides the mechanism by which hardening occurs. It may therefore be said that the ease with which dislocation are able to move, determines the degree of hardening in the material. Hence, there are two types of dislocations which should be distinguished by even the simplest dislocation model: mobile and immobile dislocations. These basic types of dislocations correspond to the basic mechanics of plastic deformation, whereby plastic strain is carried by the motion of mobile dislocations, while plastic hardening is related to the resistance from immobile dislocations. As immobile dislocations accumulate, the mobile dislocations interact to an increasing degree with immobile dislocations and movement becomes more difficult. Consequently the threshold of stress required to produce additional plastic strain is continuously raised. This may be recognized as the very effect that has been named “hardening” of a material.

That critical shear stress which is required to untangle the interacting dislocations and to induce a significant plastic deformation, is defined as the Taylor flow stress $\tau$ (Taylor, 1938). The Taylor flow stress may also be viewed as the passing stress for a mobile dislocation to glide through a forest of immobile dislocation without being trapped or pinned. The related hardening law, the Taylor hardening law relates the shear strength to the dislocation density, and represents the genesis and basis of the so-called mechanism-based strain gradient (MSG) plasticity theory (Nix and Gao, 1998; Gao et al., 1999a; Huang et al., 2000a; Hwang et al., 2002; Qiu et al., 2003; Hwang et al., 2003; Huang et al., 2004) as well as the Taylor-based nonlocal theory (TNT) of plasticity (Gao
The hardening law provides a simple description of the dislocation interaction process at the microscale. One form of Taylor’s hardening law which is generally accepted in literature is

\[ \tau = \tau_0 + \alpha Gb \sqrt{\rho_i} \]  

(1)

where \( \rho_i \) is the immobile forest dislocation density, \( G \) is the shear modulus, \( b \) is the magnitude of the Burgers vector, and \( \alpha \) is a material constant related to the crystal and grain structure and typically ranging from 0.1 to 0.5 (Ashby, 1970). Meanwhile, \( \tau_0 \) represents the stress extrapolated to a dislocation density of zero.

The immobile or forest dislocation density is generally assumed to represent the total coupling between two types of dislocations that play significant roles in the hardening mechanism. Deformation in metals enhances the formation, motion, and storage of dislocations. Storage of dislocations in turn is the cause of hardening in the material. Stored dislocations which are generated by trapping each other in a random way are commonly referred to as statistically stored dislocations (SSDs), while stored dislocations that maintain the plastic deformation incompatibilities within the polycrystal caused by nonuniform dislocation slip are called geometrically necessary dislocations (GNDs). The presence of GNDs causes additional storage of defects and increases the resistance to deformation by acting as an obstacle to the SSDs (Ashby, 1970).
Figure 1: Illustration of SSDs and GNDs

<table>
<thead>
<tr>
<th>Statistically Stored Dislocations</th>
<th>Geometrically Necessary Dislocations</th>
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Square Lattice in Pure Shear (Homogenous Plastic Strain)  
Square Lattice in Pure Bending (Non-homogenous Plastic Strain)

Figure 2: Transmission Electron Micrographs Showing Dislocations (URL: TEM)
4 THERMODYNAMIC FORMULATION OF LOCAL/CLASSICAL PLASTICITY

In order to formulate a continuum-based plasticity model, it is necessary to satisfy the axioms of equilibrium and thermodynamics. Herein is presented the principle of virtual power and the fundamental statements of irreversible thermodynamics that are used commonly in the mathematical modeling of the thermo-mechanical behavior of the material.

Henceforth, \( \| \| \) is the Euclidean norm of second rank tensors, \( (\cdot) \) stands for tensor contraction, the superimposed dot \( (\cdot) \) indicates the differentiation with respect to time \( t \), and a comma followed by an index \( j \) (e.g. \( x_{i,j} \)) denotes differentiation with respect to \( x_{j} \). The first-order gradient, divergence, curl, and Laplacian of a tensor field \( \mathbf{A} \) are defined by \( \text{div} \mathbf{A} = A_{j,j} \), \( (\text{curl} \mathbf{A})_g = e_{pq} A_{jq,p} \), \( (\nabla^2 \mathbf{A})_i = A_{ij,ik} \), and \( (\nabla \mathbf{A})_{ijk} = A_{ijk} \), respectively.

**Principle of Virtual Power**

The principle of virtual power may be defined as the assertion that, given any sub-body \( \Gamma \), the virtual power expended on \( \Gamma \) by exterior materials of bodies (i.e. external power) must be identical to the virtual power expended within \( \Gamma \) (i.e. internal power). It may be stated that the principle of virtual power is the cornerstone of the Finite Element Method.

Let \( \mathbf{n} \) denote the outward unit normal of \( \partial \Gamma \). The expenditure of external power is assumed to arise from a macroscopic surface traction \( \mathbf{t} \), a macroscopic body force \( \mathbf{b} \), and inertia forces whose virtual work is associated with the macroscopic motion of the body. This motion is defined by the virtual velocity vector \( \mathbf{v} \). The external power may therefore be written in the following form:
\[ P_{\text{ext}} = \int_{\Gamma} b v_i dV + \int_{\Gamma} t v_i dA - \int_{\Gamma} \rho v_i dV \]  

(2)

where \( \rho \) is the mass density and \( \dot{v} \) is the acceleration vector. The external power is balanced by an internal expenditure of power. The internal expenditure of power is characterized by an elastic stress \( \sigma \) defined over \( \Gamma \) for all time, the back-stress \( X \) associated with kinematic hardening, and the drag-stress \( R \) associated with isotropic hardening. The internal power is assumed to have the following form

\[ P_{\text{int}} = \int_{\Gamma} \left( \sigma_{ij} \dot{e}^e_{ij} + X_{ij} \dot{\varepsilon}^p_{ij} + R \dot{\rho} \right) dV \]  

(3)

and is also assumed to balance external power \( P_{\text{ext}} \) such that

\[ P_{\text{ext}} = P_{\text{int}} \]  

(4)

The energetic balance is better characterized by a dependence of \( P_{\text{int}} \) on the plastic strain \( \varepsilon^p \) rather than on the (scalar) accumulation of the plastic strain \( p \) (internal history variable), since a dependence of \( P_{\text{int}} \) on \( \varepsilon^p \) gives rise to kinematic hardening; while a dependence of \( P_{\text{int}} \) on \( p \) gives rise to isotropic hardening.

The second-order tensor \( \sigma \) introduced above will be shown to be the symmetric Cauchy stress tensor. Meanwhile, the second-order tensor, \( \dot{\varepsilon} \), is the rate of deformation which is defined by the symmetric part of the velocity gradient \( v_{i,j} \)

\[ \dot{e}_{ij} = \frac{1}{2} \left(v_{i,j} + v_{j,i}\right) \]  

(5)

The classical theory of small deformation isotropic plasticity is based on the additive decomposition of the total strain rate into elastic and plastic parts, with \( \dot{\varepsilon}^e \) being the elastic component and \( \dot{\varepsilon}^p \) being the corresponding plastic component such that:
\[ \dot{\varepsilon}_{ij} = \dot{\varepsilon}^e_{ij} + \dot{\varepsilon}^p_{ij}, \quad \dot{\varepsilon}^p_{kk} = 0 \]  

(6)

where the superscripts \( e \) and \( p \) denote the elastic and plastic parts, respectively. The second term in Eq. (3) represents the internal power associated with the back-stress \( \mathbf{X} \), which is attributed to kinematic hardening. The kinematic variable used most commonly in classical nonlocal plasticity is the plastic strain itself (\( \varepsilon^p \)). An example of this is Prager’s hardening model, which is a linear kinematic hardening model. A more general flux tensor associated with back-stress, the Frederick-Armstrong evanescent memory kinematic flux, will be used in the following section and in the higher-order nonlocal formulation. The third term in Eq. (3) represents the internal power associated with the drag-stress \( \mathbf{R} \) which causes isotropic hardening. The variable \( p \) is defined as the accumulated or effective plastic strain and its rate is defined by the expression

\[ \dot{p} = \| \dot{\varepsilon}^p_{ij} \| = \sqrt{\dot{\varepsilon}^p_{ij} \dot{\varepsilon}^p_{ij}} \]  

(7)

Furthermore, the unit direction of the plastic strain may be defined as

\[ N_{ij} = \frac{\dot{\varepsilon}^p_{ij}}{\| \dot{\varepsilon}^p_{ij} \|} = \frac{\dot{\varepsilon}^p_{ij}}{\dot{p}} \]  

(8)

In this way one may write

\[ \| N_{ij} \| N_{ij} N_{ij} = 1 \Rightarrow N_{ij} \frac{\dot{\varepsilon}^p_{ij}}{\dot{p}} = 1 \Rightarrow N_{ij} \dot{\varepsilon}^p_{ij} = \dot{p} \Rightarrow \dot{\varepsilon}^p_{ij} = \dot{p} N_{ij} \]  

(9)

with the last expression corresponding to the definition of the flow rule in classical plasticity theory.

If the axiom of equilibrium of the principle of virtual power is applied to the region \( \Gamma \), Eq.(4), the following equilibrium equation is obtained
\begin{equation}
\int b_j \nu_j dV + \int t_i \nu_i dA - \int \rho \dot{\nu}_i \nu_i dV = \int \left( \sigma_{ij} \dot{\varepsilon}_{ij} + X_{ij} \dot{\varepsilon}^p_{ij} + R \dot{p} \right) dV
\end{equation}

(10)

Substituting both Eq. (9) and Eq. (6) into the above expression yields

\begin{equation}
\int b_j \nu_j dV + \int t_i \nu_i dA - \int \rho \dot{\nu}_i \nu_i dV = \int \left[ \sigma_{ij} \dot{\varepsilon}_{ij} - \left( \tau_{ij} - X_{ij} - R N_{ij} \right) \dot{\varepsilon}^p_{ij} \right] dV
\end{equation}

(11)

where, due to plastic incompressibility, it can easily be proven that $\sigma : \dot{\varepsilon}^p = \tau : \dot{\varepsilon}^p$ where $\tau_{ij} = \sigma_{ij} - \frac{1}{3} \sigma_{kk} \delta_{ij}$ is the deviatoric component of the Cauchy stress tensor, $\sigma$. By applying the divergence theorem (also known as Gauss’ theorem or integration by parts), the following expression may be derived

\begin{equation}
\int \sigma_{ij} \dot{\varepsilon}_{ij} dV = \int \sigma_{ij} \nu_{i,j} dV = \int \left( \sigma_{ij} \nu_i \right)_j dV - \int \sigma_{ij} \nu_{i,j} dV
\end{equation}

\begin{equation}
= \int \sigma_{ij} \nu_i dA - \int \sigma_{ij} \nu_{i,j} dV
\end{equation}

(12)

and Eq. (11) may be rewritten as

\begin{equation}
\int \left( \sigma_{ij,i} + b_i - \rho \dot{v}_i \right) \nu_i dV + \int \left( t_i - \sigma_{ij} n_j \right) \nu_i dA + \int \left( \tau_{ij} - X_{ij} - R N_{ij} \right) \dot{\varepsilon}^p_{ij} dV = 0
\end{equation}

(13)

$\Gamma$, $\nu$, and $\dot{\varepsilon}^p$ may be arbitrarily specified if and only if

\begin{equation}
\sigma_{ij,i} + b_i = \rho \dot{v}_i \quad \text{(macro-force balance)}
\end{equation}

(14)

\begin{equation}
t_i = \sigma_{ij} n_j \quad \text{(macro-traction condition)}
\end{equation}

(15)

and

\begin{equation}
\tau_{ij} - X_{ij} - R N_{ij} = 0 \quad \text{(micro-force balance)}
\end{equation}

(16)

In the first of these three equations, the local static or dynamic equilibrium or the macro-force balance is expressed according to the notion of Gurtin (2003). In the second one the stress vector is defined as the surface density of the forces introduced. It is shown that $\sigma$ is really the Cauchy stress tensor, which is a second-order symmetric tensor. It
also provides the local macro-traction boundary conditions on forces if the axiom of equilibrium of virtual power is applied to the whole region under consideration as opposed to arbitrarily sub-regions.

**Local Yield Criterion**

Meanwhile the third of the equations above, Eq.(16), represents the micro-force balance. It can easily be shown that this micro-force balance is nothing more than the yield criterion of classical plasticity theory. Substituting Eq. (8) into Eq. (16), one can write the following expression for the flow rule, Eq. (9)4:

\[
N_{ij} = \frac{\tau_{ij} - X_{ij}}{R} \Rightarrow \dot{\epsilon}_{ij}^p = \frac{\dot{p} \tau_{ij} - X_{ij}}{R}
\]  

(17)

Furthermore, by taking the Euclidean norm \( \| \) of Eq. (16) one can write

\[
\| \tau_{ij} - X_{ij} \| N_{ij} - R = 0
\]

(18)

However, since \( \| N_{ij} \| = 1 \) and \( \| R \| = R \), the following expression can be written

\[
\| \tau_{ij} - X_{ij} \| - R = 0
\]

(19)

This equation constitutes the von-Mises yield criterion of local plasticity. Therefore, the micro-force balance, Eq. (18), may be set as the yield criterion or the plasticity loading surface \( f \)

\[
f = \| \tau_{ij} - X_{ij} \| - R = 0
\]

(20)

such that the flow rule in Eq. (17) can also be expressed by

\[
\dot{\epsilon}_{ij}^p = \frac{\dot{p} \tau_{ij} - X_{ij}}{\| \tau_{mn} - X_{mn} \|}
\]

(21)
Comparing Eq. (21) with Eq. (8), it is possible to reformulate the direction of the plastic flow as

\[ N_{ij} = \frac{\tau_{ij} - X_{ij}}{\|\tau_{mn} - X_{mn}\|} \]  

(22)

It is obvious that Eq. (20) represents a sphere in deviatoric stress-space of radius \( R \) centered at \( \mathbf{X} \). The radius \( R \) represents isotropic hardening while the backstress \( \mathbf{X} \) represents kinematic hardening. Furthermore, the flow rule in Eq. (21) dictates that the flow direction \( \mathbf{N} \) in Eq. (22) is normal to the yield surface and directed outward from the yield surface.

Remark: The micro-force balance from the principal of virtual power represents the yield criterion or the yield function in the theory of plasticity.

**Local Clausius-Duhem Inequality**

Using the conclusion above, it can easily be proved that the internal virtual power in Eq. (3), after substituting Eqs. (6)1, (9)3, and (16), can be rewritten as

\[ P_{int} = \int_{\Gamma} \sigma_{ij} \dot{\varepsilon}_{ij} dV \]  

(23)

This expression coincides with the classical definition by Green and Naghdi (1971).

The macro-force balance equation, Eq. (14), can be interpreted as a form of the law of conservation of momentum. By integrating it over \( \Gamma \) and applying the divergence theorem along with Eq. (15), the global mechanical conservation law is obtained as

\[ \int_{\partial \Gamma} t_i dA + \int_{\Gamma} h_i dV = \frac{d}{dt} \int_{\Gamma} \rho v_i dV \]  

(24)

with \( d/dt \) denoting the material derivative.
Similarly, the symmetry of the Cauchy stress tensor, $\sigma_{ij} = \sigma_{ji}$, which results directly from the principle of virtual power, can be considered to be a consequence of the equation of momentum balance equation. Furthermore, the conservation of mass law can be obtained as

$$\frac{d}{dt} \int_{V} \rho dV = 0$$  \hspace{1cm} (25)

The main consideration here is a purely mechanical theory (isothermal conditions are assumed) based on the requirement that the rate of change in the total free energy should be less than or equal to the work of external forces (Gurtin, 2002). If the specific free energy is denoted as $\rho \Psi$, this requirement takes the form of a free energy inequality

$$\int_{V} \rho \Psi dV \leq P_{ext}$$  \hspace{1cm} (26)

From Eq. (25) it is possible to write $\int_{V} \rho \Psi dV = \int_{V} \rho \dot{\Psi} dV$. Furthermore, substituting the virtual work balance equation, Eq. (4), into Eq. (26) along with the new form of the internal power presented in Eq.(23), one can write the following thermodynamic restriction

$$\sigma_{ij} \dot{\varepsilon}_{ij} - \rho \dot{\Psi} \geq 0$$  \hspace{1cm} (27)

The reader will recognize this as the classical (local) Clausius-Duhem inequality.

The degree of precision with which material plasticity can be described is dependent upon the choice of the nature and the number of state variables. The processes of plasticity will be admissible if, at any instant of the evolution, the Clausius-Duhem inequality is satisfied. The state variables, also called thermodynamic or independent
variables, are the observable and the internal variables. The particular state variables to use are chosen based on the application and purpose of the model.

**Local State Variables**

Hardening in plasticity is introduced by hidden independent internal state variables in the thermodynamic state potential. The Helmholtz free specific energy can be considered as the thermodynamic state potential which depends on both observable and internal state variables. In order to define the Helmholtz free specific energy, it is necessary to choose the nature of the state variables. The choice made here is a classical form of this potential in terms of the elastic strain, $\varepsilon^e$, and $n_{\text{int}}$ - of phenomenological dissipative internal state variables ($\mathcal{N}_k$, $k = 1, \ldots, n_{\text{int}}$; $n_{\text{int}} \geq 1$):

$$\Psi = \tilde{\Psi} \left( \varepsilon^e_{ij}, \mathcal{N}_k \right)$$  \hspace{1cm} (28)

In order to incorporate the plasticity isotropic and kinematic hardening effects, a finite set of internal state variables $\mathcal{N}_k$ ($k = 1, \ldots, n_{\text{int}}$) representing either scalars or tensorial variables are assumed such that

$$\mathcal{N}_k = \mathcal{N}_k \left( \varepsilon^p_{ij}, p \right)$$  \hspace{1cm} (29)

where $\varepsilon^p$ and $p$ are internal variables characterize the kinematic and isotropic and hardening flux variables in classical plasticity, respectively. Moreover, the free energy in Eq. (28) is assumed to have the following decoupled form

$$\Psi = \Psi^e \left( \varepsilon^e_{ij} \right) + \Psi^p \left( \varepsilon^p_{ij}, p \right)$$  \hspace{1cm} (30)

where $\Psi^e$ is the elastic energy and $\Psi^p$ is the plastic energy. This assumption classifies the material as a *separable material* (Gurtin, 2003) whereby there is no interaction between the stretching of the material structure as characterized by the elastic strain $\varepsilon^e$
and the evolution and interaction of dislocations and other defects as characterized by $\varepsilon^p$ and $p$.

The time derivative of Eq. (28) with respect to its internal state variables in Eq. (29) is given by the expression:

$$\dot{\Psi} = \frac{\partial \Psi^e}{\partial \varepsilon^e_{ij}} \dot{\varepsilon}^e_{ij} + \frac{\partial \Psi^p}{\partial \varepsilon^p_{ij}} \dot{\varepsilon}^p_{ij} + \frac{\partial \Psi^p}{\partial p} \dot{p} = \frac{\partial \Psi^e}{\partial \varepsilon^e_{ij}} \dot{\varepsilon}^e_{ij} + \left( \frac{\partial \Psi^p}{\partial \varepsilon^p_{ij}} + \frac{\partial \Psi^p}{\partial p} N_{ij} \right) \dot{\varepsilon}^p_{ij}$$

(31)

where Eq. (8) is used. Substitution of Eq. (31) into the Clausius-Duhem inequality, Eq. (27), yields the following expression:

$$\left( \sigma_{ij} - \rho \frac{\partial \Psi^e}{\partial \varepsilon^e_{ij}} \right) \dot{\varepsilon}^e_{ij} + \left( \tau_{ij} - \rho \frac{\partial \Psi^p}{\partial \varepsilon^p_{ij}} - \rho \frac{\partial \Psi^p}{\partial p} N_{ij} \right) \dot{\varepsilon}^p_{ij} \geq 0$$

(32)

A classical hypothesis permits the cancellation of some terms in this inequality independently from which the following thermodynamic state laws are obtained

$$\sigma_{ij} = \rho \frac{\partial \Psi^e}{\partial \varepsilon^e_{ij}}$$

(33)

$$J_{ij} = \tau_{ij} - \rho \frac{\partial \Psi^p}{\partial \varepsilon^p_{ij}} - \rho \frac{\partial \Psi^p}{\partial p} N_{ij}$$

(34)

**Local Plastic Flow Rule**

By substituting the thermodynamic state laws, Eqs. (33) and (34), back into the Clausius-Duhem inequality, Eq. (32), one obtains

$$\Pi = J_{ij} \dot{\varepsilon}^p_{ij} \geq 0$$

(35)

where $\Pi$ is the dissipation energy per unit volume. Substituting the expression for $\dot{\varepsilon}^p_{ij}$ from Eq. (9), into Eq. (35) and defining

$$\gamma = J_{ij} N_{ij} \geq 0$$

(36)
yields the following

$$\Pi = \gamma \dot{p} \geq 0$$  \hspace{1cm} (37)

where $\gamma = \Pi / \dot{p} > 0$ for $\dot{p} > 0$ can be interpreted as the *dissipation modulus* (Gurtin, 2003). Further, one obtains $\gamma = 0$ for $\dot{p} = 0$. Equating Eqs. (35) and (37) yields

$$\gamma \dot{p} = J_y \dot{E}_y^p \Rightarrow \gamma = J_y N_y \Rightarrow \gamma = \|J_y\| \Rightarrow \gamma = \|J_y\|$$  \hspace{1cm} (38)

Thus one can write the plastic flow direction $N$ from Eq. (38)_4 and Eq. (36) as

$$N_{ij} = \frac{J_{\dot{y}}}{\|J_y\|}$$  \hspace{1cm} (39)

Therefore from Eqs. (39), (38), and (34) one can write the flow direction as

$$N_{ij} = \frac{\tau_{ij} - \rho \frac{\partial \Psi^p}{\partial \epsilon_{ij}^p}}{\gamma + \rho \frac{\partial \Psi^p}{\partial \phi}}$$  \hspace{1cm} (40)

Comparing Eqs. (39) and (22), one can write

$$J_y = \tau_y - X_y \Rightarrow \|J_y\| = \|\tau_y - X_y\|$$  \hspace{1cm} (41)

Equating Eqs. (41)_1 and (34), or equivalently comparing Eqs. (40) and (17)_1, yields the following expression for the back-stress $X$

$$X_{ij} = \rho \frac{\partial \Psi^p}{\partial \epsilon_{ij}^p}$$  \hspace{1cm} (42)

Moreover, comparing Eqs. (41)_2, (38), and (20)_1 gives the micro-force $R$ as

$$R = \gamma + \rho \frac{\partial \Psi^p}{\partial \phi}$$  \hspace{1cm} (43)

From the above equation it appears that the isotropic hardening/softening function $R$ is the sum of a dissipative term $\gamma > 0$ and an energetic term $\rho \frac{\partial \Psi}{\partial \phi}$. The conjugate
force $R$ has a hardening or softening effect as $\rho \partial \Psi / \partial p > 0$ or $< 0$, respectively.

A direct consequence of the above formalism is that the yield function in Eq. (20) can be derived from the principle of virtual power. This yield surface is spherical in the deviatoric stress space of radius $R$ and centered at the back-stress $X$. Moreover, the direction of the plastic flow $N$ is normal to the yield surface and directed outward.

**The Principle of Maximum Dissipation**

The maximum dissipation principle (also principle of maximum entropy production) states that the physical state of the thermodynamic forces is the one that maximizes the dissipation function over all other possible admissible states. This principle is a central pillar of the mathematical formulation of plasticity (Duvat and Lions, 1972).

From the previous discussion it can be observed that the thermodynamic potential $\Psi$ allows one to write relations between internal variables and the corresponding conjugate forces. However, in order to describe the dissipation process the evolution of the internal variables is needed, which can be obtained through the use of the generalized normality rule of thermodynamics which is a consequence of the maximum dissipation principle. In this regard the evolution laws for the plastic strain rate, $\dot{\varepsilon}^p$, and the rate of the isotropic hardening flux, $\dot{\rho}$, can be obtained by utilizing the calculus of function of several variables with the Lagrange multiplier, $\lambda$, and subjected to a constrain $f = 0$ from Eq. (20). Formulating this principle, the objective function $\Omega$ can be constructed in the following form:

$$\Omega = -\Pi + \dot{\lambda} f$$

(44)

In order to obtain $\dot{\varepsilon}^p$ and $\dot{\rho}$, the following conditions are used to maximize the objective function, $\Omega$, respectively:
\[
\frac{\partial \Omega}{\partial J_{ij}} = 0 \Rightarrow \frac{\partial \Omega}{\partial \sigma_{ij}} = 0, \quad \frac{\partial \Omega}{\partial X_{ij}} = 0, \quad \frac{\partial \Omega}{\partial R} = 0
\]  
(45)

By Substituting Eq. (35) into the above relations along with Eq. (34) and Eqs. (42) and (43), the corresponding flow rules of \( \dot{\varepsilon}^p \) and \( \dot{p} \) are obtained, respectively, as follows:

\[
\dot{\varepsilon}^p_{ij} = \lambda \frac{\partial f}{\partial J_{ij}} \Rightarrow \dot{\varepsilon}^p_{ij} = \dot{\lambda} \frac{\partial f}{\partial \sigma_{ij}}, \quad \dot{X}_{ij} = \dot{\lambda} \frac{\partial f}{\partial X_{ij}}, \quad \dot{p} = -\dot{\lambda} \frac{\partial f}{\partial R} = \dot{\lambda}
\]  
(46)

where \( \dot{\lambda} \) is the plastic multiplier which can be determined from the Kuhn-Tucker loading/unloading conditions

\[
f \leq 0, \quad \dot{\lambda} \geq 0, \quad \dot{\lambda} f = 0 \quad \text{and} \quad \dot{\lambda} \dot{f} = 0
\]  
(47)

It can be noted that the whole problem of modeling the plasticity phenomenon lies in the determination of the analytical expressions for the Helmholtz free energy function \( \Psi \) and its identification from experiments.
5 THERMODYNAMIC FORMULATION IN LOCAL PLASTICITY WITH ANISOTROPIC HARDENING

Kinematic Flux Expression

Zbib and Aifantis (1988) indicated that the plastic spin is a consequence of standard kinematic arguments in conjunction with the constitutive equation for the rate of plastic deformation $\dot{\varepsilon}_{ij}^p$. Aifantis (1984) and Zbib and Aifantis (1988) used the single slip theory and showed that the evolution equation for the back stress flux $\alpha_{ij}$ is given by

$$\dot{\alpha}_{ij} = (i_m t_m - i_n t_n) \dot{\varepsilon}_{ij}^p + \frac{i_n}{t_n} \alpha$$

where $t_m$ and $t_n$ are scalar functions of $\gamma^n$, and $\dot{\gamma}^p$ is the rate of shearing of the slip system. Based on the growth law in Eq. (48), several evolution equations for the back stress were derived by Zbib and Aifantis (1988). The first type is obtained by setting

$$t_n = -\frac{1}{\zeta} = \text{const} \tan t$$

Equation (48) along with Equation (49) lead to the well-known Prager kinematic hardening rule. The corresponding plastic spin in this case is obtained from Eq. (48) by using the constant value of $l$ in Eq. (49). A second type of evolution is obtained from Equation (48) by assuming

$$t_n = \frac{-1}{\zeta} e^{-c \gamma^p}$$

$$t_n = \frac{k}{c_n} \frac{1}{\zeta_0} e^{-c \gamma^p}$$

where $c$ and $k$ are constants. These equations will lead to the Armstrong-Frederick evanescent memory kinematic hardening evolution equation for the backstress.
\[ \dot{\alpha} = k \dot{\varepsilon}^p - c\dot{p}\alpha \]  \hspace{1cm} (52)

In this case the resulting equation for the plastic spin contains an exponential term as follows:

\[ W^p = \zeta \varepsilon^p \alpha (\alpha \varepsilon^p - \varepsilon^p \alpha) \]  \hspace{1cm} (53)

Expression (49), which is used in conjunction with Eq. (6) may be further generalized such that it may be used with the more general expression (5) for the plastic spin tensor.

**Principle of Virtual Power**

The external power is written as before

\[ P_{\text{ext}} = \int b_i v_i dV + \int t_i v_i dA - \int \rho \dot{v}_i V_i dV \]  \hspace{1cm} (54)

where, again, \( \rho \) is the mass density and \( \dot{v} \) is the acceleration vector. The external power is balanced by the internal expenditure of power. The internal expenditure of power is characterized by the elastic stress \( \sigma \) defined over \( \Gamma \) for all time, the back-stress \( X \) associated with kinematic hardening, and the drag-stress \( R \) associated with isotropic hardening. The internal power is now assumed to have the following form

\[ P_{\text{int}} = \int (\sigma_{ij} \dot{\varepsilon}^e_{ij} + X_{ij} \dot{\alpha}_{ij} + R \dot{p}) dV \]  \hspace{1cm} (55)

where the kinematic flux \( \dot{\alpha} \) is defined by the expression from Equation (52), that is

\[ \dot{\alpha} = k \dot{\varepsilon}^p - c\dot{p}\alpha . \]  

Internal power is balanced by external power \( P_{\text{ext}} \) such that

\[ P_{\text{ext}} = P_{\text{int}} \]  \hspace{1cm} (56)

As before, the rate of deformation is defined by

\[ \dot{\varepsilon}_{ij} = \frac{1}{2} \left( v_{i,j} + v_{j,i} \right) \]  \hspace{1cm} (57)
Also the additive decomposition of the total strain rate into elastic and plastic parts, is assumed, such that:

$$\dot{\varepsilon}_{ij} = \dot{\varepsilon}_{ij}^e + \dot{\varepsilon}_{ij}^p, \quad \dot{\varepsilon}_{kk}^p = 0$$  \hspace{1cm} (58)

The more general flux tensor used here, the Frederick-Armstrong evanescent memory kinematic flux, introduces anisotropy to the hardening formulation. The rate of the accumulated plastic strain is still defined using plastic strain

$$\dot{\p} = \left\|\dot{\varepsilon}_{ij}^p\right\| = \sqrt{\dot{\varepsilon}_{ij}^p \dot{\varepsilon}_{ij}^p}$$  \hspace{1cm} (59)

also the unit direction of the plastic strain is defined as

$$N_{ij} = \frac{\dot{\varepsilon}_{ij}^p}{\left\|\dot{\varepsilon}_{ij}^p\right\|} = \frac{\dot{\varepsilon}_{ij}^p}{\dot{\p}}$$  \hspace{1cm} (60)

So that one may still write

$$\left\|N_{ij}\right\| = N_{ij} N_{ij} = 1 \Rightarrow N_{ij} \frac{\dot{\varepsilon}_{ij}^p}{\dot{\p}} = 1 \Rightarrow N_{ij} \dot{\varepsilon}_{ij}^p = \dot{\p} \Rightarrow \dot{\varepsilon}_{ij}^p = \dot{\p} N_{ij}$$  \hspace{1cm} (61)

The axiom of equilibrium of the principle of virtual power is applied to the region $\Gamma$, Eq. (56), and the equilibrium equation becomes

$$\int_{\Gamma} \left[ b_i v_i dV + \int_{\Gamma} t_i v_i dA - \int_{\Gamma} \rho \dot{v}_i v_i dV = \int_{\Gamma} \left( \sigma_{ij} \dot{\varepsilon}_{ij}^e + X_{ij} \dot{\alpha}_{ij} + R \dot{\p} \right) dV \right]$$  \hspace{1cm} (62)

Substituting both Eq. (61) and from Eq. (58), $\dot{\varepsilon}^e = \dot{\varepsilon} - \dot{\varepsilon}^p$ into the above expression yields

$$\int_{\Gamma} \left[ b_i v_i dV + \int_{\Gamma} t_i v_i dA - \int_{\Gamma} \rho \dot{v}_i v_i dV = \int_{\Gamma} \left\{ \sigma_{ij} \dot{\varepsilon}_{ij} - \left[ \tau_{ij} - k X_{ij} - \left( R - c X_{mn} \alpha_{mn} \right) N_{ij} \right] \dot{\varepsilon}_{ij}^p \right\} dV \right]$$  \hspace{1cm} (63)
where, due to plastic incompressibility $\sigma : \dot{\varepsilon}^p = \tau : \dot{\varepsilon}^p$ with $\tau_{ij} = \sigma_{ij} - \frac{1}{3} \sigma_{kk} \delta_{ij}$ is the deviatoric component of the Cauchy stress tensor, $\sigma$. Applying the divergence theorem, the following expression is derived

$$\int \sigma_{y} \dot{\varepsilon}_{y} dV = \int \sigma_{y} v_{i,j} dV = \int (\sigma_{y} v_{i})_{,j} dV - \int \sigma_{y,j} v_{i} dV = \int_{\partial V} \sigma_{y,n} v_{i} dA - \int \sigma_{y,j} v_{i} dV$$

and Eq. (63) may be rewritten as

$$\int (\sigma_{y,j} + b_{i} - \rho \dot{v}_{i}) v_{i} dV + \int (t_{i} - \sigma_{y,n} n_{j}) v_{i} dA$$

$$+ \int \left[ \tau_{ij} - kX_{ij} - \left( R - cX_{mn} \alpha_{mn} \right) N_{ij} \right] \dot{\varepsilon}_{y} dV = 0$$

$\Gamma$ , $v$ , and $\dot{\varepsilon}^p$ may be arbitrarily specified if and only if

$$\sigma_{y,j} + b_{i} = \rho \dot{v}_{i} \quad (macro-force balance) \tag{66}$$

$$t_{i} = \sigma_{y,n} n_{j} \quad (macro-traction condition) \tag{67}$$

and

$$\tau_{ij} - kX_{ij} - RN_{ij} + cX_{mn} \alpha_{mn} N_{ij} = 0 \quad (micro-force balance) \tag{68}$$

**Local Yield Criterion**

Once again, the micro-force balance can be shown to be nothing more than the yield criterion of classical plasticity theory. Substituting Eq. (60) into Eq. (68), it is possible to write the following expression for the flow rule, Eq. (61):

$$N_{ij} = \frac{\tau_{ij} - kX_{ij}}{R - cX_{mn} \alpha_{mn}} \Rightarrow \dot{\varepsilon}_{yi}^p = \dot{\rho} \frac{\tau_{ij} - kX_{ij}}{R - cX_{mn} \alpha_{mn}}$$

Taking the Euclidean norm $\| \|$ of Eq. (68) one can write

$$\| \tau_{ij} - kX_{ij} \| - \| R - cX_{mn} \alpha_{mn} \| N_{ij} = 0 \tag{70}$$
And, since $\|N_{ij}\| = 1$ and $\| R \| = R$, the von-Mises yield criterion can be written

$$\| \tau_{ij} - kX_{ij} \| - mR = 0$$

(71)

Therefore, the micro-force balance, Eq. (70), may be set as the yield criterion or the plasticity loading surface $f$

$$f = \| \tau_{ij} - kX_{ij} \| - mR = 0$$

(72)

such that the flow rule in Eq. (69) can also be expressed by

$$\dot{\epsilon}_{ij}^p = \dot{\rho} \frac{\tau_{ij} - kX_{ij}}{\| \tau_{mn} - kX_{mn} \|}$$

(73)

Comparing Eq. (73) with Eq. (60), it is possible to reformulate the direction of the plastic flow as

$$N_{ij} = \frac{\tau_{ij} - kX_{ij}}{\| \tau_{mn} - kX_{mn} \|}$$

(74)

It is obvious that Eq. (72) represents a sphere in deviatoric stress-space of radius $R$ centered at $kX$. The radius $mR$ represents isotropic hardening while the backstress $kX$ represents kinematic hardening. Furthermore, the flow rule in Eq. (73) dictates that the flow direction $N$ in Eq. (74) is normal to the yield surface and directed outward from the yield surface.

**Clausius-Duhem Inequality**

The internal virtual power in Eq.(55), after substituting Eqs. (58), (61), and (68), is rewritten as

$$P_{int} = \int \sigma_{ij} \dot{\epsilon}_{ij} dV$$

(75)
Integrating the macro-force balance equation, Eq. (66) over $\Gamma$ and applying the divergence theorem along with Eq. (67)

$$\int_{\Gamma} t_t dA + \int_{\Gamma} b_j dV = \frac{d}{dt} \int_{\Gamma} \rho \Psi dV$$

(76)

The conservation of mass law is obtained as

$$\frac{d}{dt} \int_{\Gamma} \rho dV = 0$$

(77)

The rate of change in the total free energy should be less than or equal to the work of external forces (Gurtin, 2002). The specific free energy is denoted as $\rho \Psi$ so that the free energy inequality is written as

$$\int_{\Gamma} \rho \Psi dV \leq P_{ext}$$

(78)

From Eq. (77) it is possible to write $\int_{\Gamma} \rho \Psi dV = \int_{\Gamma} \rho \Psi dV$. Substituting the virtual work balance equation, Eq. (56), into Eq. (78) along with the new form of the internal power presented in Eq. (75), one can write the following thermodynamic restriction

$$\sigma_{ij} \dot{e}_{ij} - \rho \Psi \geq 0$$

(79)

**Local State Variables**

As before, the choice with regard to the Helmholtz free energy is a classical form of the thermodynamic state potential in terms of the elastic strain, $\varepsilon^e$, and $n_{int}$ - of phenomenological dissipative internal state variables ($N_k, k=1,...,n_{int}; n_{int} \geq 1$):

$$\Psi = \tilde{\Psi} \left( e^e_{ij}, N_k \right)$$

(80)
The plasticity isotropic and kinematic hardening effects are incorporated using the finite set of internal state variables $\mathbb{N}_k$ \((k = 1, \ldots, n_{\text{int}})\) representing either scalars or tensorial variables as below

$$\mathbb{N}_k = \mathbb{N}_k (\alpha_{ij}, p)$$  \hspace{1cm} (81)

where \(\alpha\) characterizes the kinematic hardening flux variable and \(p\) the hardening flux variable in classical plasticity. Therefore the free energy in Eq. (80) can be assumed to have the following decoupled form

$$\Psi = \Psi^e (\varepsilon_{ij}^e) + \Psi^p (\alpha_{ij}, p)$$  \hspace{1cm} (82)

where, using the separable material characterization, \(\Psi^e\) is the elastic energy and \(\Psi^p\) is the plastic energy.

The time derivative of Eq. (80) with respect to its internal state variables in Eq. (81) is now given by the expression:

$$\dot{\Psi} = \frac{\partial \Psi^e}{\partial \varepsilon_{ij}^e} \dot{\varepsilon}_{ij}^e + \frac{\partial \Psi^p}{\partial \alpha_{ij}} \dot{\alpha}_{ij} + \frac{\partial \Psi^p}{\partial p} \dot{p}$$

$$\dot{\Psi} = \frac{\partial \Psi^e}{\partial \varepsilon_{ij}^e} \dot{\varepsilon}_{ij}^e + \left[ k \frac{\partial \Psi^p}{\partial \alpha_{ij}} + \left( \frac{\partial \Psi^p}{\partial p} - c \frac{\partial \Psi^p}{\partial \alpha_{pq}} \alpha_{pq} \right) N_{ij} \right] \dot{\varepsilon}_{ij}^p$$  \hspace{1cm} (83)

where Eq. (60) is used. Substitution of Eq. (83) into the Clausius-Duhem inequality, Eq. (79), yields the following expression:

$$\left( \sigma_{ij} - \rho \frac{\partial \Psi^e}{\partial \varepsilon_{ij}^e} \right) \dot{\varepsilon}_{ij}^e + \left( \tau_{ij} - \rho \left[ k \frac{\partial \Psi^p}{\partial \alpha_{ij}} + \left( \frac{\partial \Psi^p}{\partial p} - c \frac{\partial \Psi^p}{\partial \alpha_{pq}} \alpha_{pq} \right) N_{ij} \right] \right) \dot{\varepsilon}_{ij}^p \geq 0$$  \hspace{1cm} (84)

A classical hypothesis permits the cancellation of some terms in this inequality independently from which the following thermodynamic state laws are obtained
\[ \sigma_{ij} = \rho \frac{\partial \Psi^e}{\partial \varepsilon_{ij}^e} \]  \hspace{1cm} (85)

\[ J_{ij} = \tau_{ij} - \rho \left[ k \frac{\partial \Psi^p}{\partial \alpha_{ij}} + \left( \frac{\partial \Psi^p}{\partial p} - c \frac{\partial \Psi^p}{\partial \alpha_{pq}} \alpha_{pq} \right) N_{ij} \right] \]  \hspace{1cm} (86)

**Local Plastic Flow Rule**

By substituting the thermodynamic state laws, Eqs. (85) and (86), back into the Clausius-Duhem inequality, Eq. (84), the following expression is obtained

\[ \Pi = J_{ij} \dot{\varepsilon}_{ij}^p \geq 0 \]  \hspace{1cm} (87)

where \( \Pi \) is the dissipation energy per unit volume. Substituting the expression for \( \dot{\varepsilon}_{ij}^p \) from Eq. (61) into Eq. (87) and defining

\[ \gamma = J_{ij} N_{ij} \geq 0 \]  \hspace{1cm} (88)

yields the following

\[ \Pi = \gamma \dot{p} \geq 0 \]  \hspace{1cm} (89)

where \( \gamma = \Pi / \dot{p} > 0 \) for \( \dot{p} > 0 \) can be interpreted as the *dissipation modulus* (Gurtin, 2003). Further, one obtains \( \gamma = 0 \) for \( \dot{p} = 0 \). Equating Eqs. (87) and (89) yields

\[ \gamma \dot{p} = J_{ij} \dot{\varepsilon}_{ij}^p \Rightarrow \gamma = J_{ij} N_{ij} \Rightarrow \gamma = \| J_{ij} \| N_{ij} \Rightarrow \gamma = \| J_{ij} \| \]  \hspace{1cm} (90)

Thus it is possible to write the plastic flow direction \( \mathbf{N} \) from Eq. (90) and Eq. (88) as

\[ N_{ij} = \frac{J_{ij}}{\| J_{ij} \|} \]  \hspace{1cm} (91)

Therefore from Eqs. (91), (90), and (86) the flow direction may now be written as
Comparing Eqs. (91) and (74), the following expression may be written

\[ J_{ij} = \tau_{ij} - kX_{ij} \Rightarrow \left\| J_{ij} \right\| = \left\| \tau_{ij} - kX_{ij} \right\| \]  

(93)

Equating Eqs. (93)1 and (86), or comparing Eqs. (92) and (69)1, yields this new expression for the back-stress \( X \)

\[ X_{ij} = \rho \frac{\partial \Psi}{\partial \alpha_{ij}} \]  

(94)

Furthermore, comparison of Eqs. (93)2, (90), and (72)1 yields the new micro-force \( R \) as

\[ R = \gamma + \rho \frac{\partial \Psi}{\partial p} \]  

(95)

\[ R = \frac{\gamma}{m} + \rho \left( \frac{\partial \Psi}{\partial p} - c \frac{\partial \Psi}{\partial \alpha_{pq}} \alpha_{pq} \right) \]  

(96)

From the above equation it appears that the isotropic hardening/softening function \( R \) is the sum of a dissipative term \( \gamma > 0 \) and an energetic term \( \frac{\rho}{m} \left( \frac{\partial \Psi}{\partial p} - c \frac{\partial \Psi}{\partial \alpha_{pq}} \alpha_{pq} \right) \). The conjugate force \( R \) has a hardening or softening effect as \( \frac{\rho}{m} \left( \frac{\partial \Psi}{\partial p} - c \frac{\partial \Psi}{\partial \alpha_{pq}} \alpha_{pq} \right) > 0 \) or \( < 0 \), respectively.

As a consequence of the above, the yield function in Eq. (72) may be derived from the principle of virtual power. This yield surface is spherical in the deviatoric stress space of radius \( mR \) and centered at the back-stress \( kX \). Additionally, the direction of the
plastic flow \( N \) is normal to the yield surface and outwardly directed.

**The Principle of Maximum Dissipation**

Formulating the principle as before, the objective function \( \Omega \) can be constructed in the following form:

\[
\Omega = -\Pi + \dot{\lambda} f
\]  

(97)

In order to obtain \( \dot{\epsilon}^p \) and \( \dot{\alpha} \), the following conditions are used to maximize the objective function, \( \Omega \), respectively:

\[
\frac{\partial \Omega}{\partial J_{ij}} = 0 \Rightarrow \frac{\partial \Omega}{\partial \sigma_{ij}} = 0, \quad \frac{\partial \Omega}{\partial X_{ij}} = 0, \quad \frac{\partial \Omega}{\partial \lambda} = 0
\]  

(98)

Substituting Eq. (87) into the above relations along with Eq. (86) and Eqs. (94) and (95), the corresponding flow rules of \( \dot{\epsilon}^p \), \( \dot{\alpha} \), and \( \dot{\lambda} \) are obtained, respectively, as follows:

\[
\dot{\epsilon}_{ij}^p = \dot{\lambda} \frac{\partial f}{\partial J_{ij}} \Rightarrow \dot{\epsilon}_{ij}^p = \dot{\lambda} \frac{\partial f}{\partial \sigma_{ij}}, \quad \dot{\alpha}_{ij} = -\frac{\dot{\lambda}}{k} \frac{\partial f}{\partial X_{ij}}, \quad \dot{\lambda} = \frac{\partial f}{\partial \lambda} \quad \text{and} \quad \dot{\lambda} \dot{f} = 0
\]  

(99)

where \( \dot{\lambda} \) is the plastic multiplier which can be determined from the Kuhn-Tucker loading/unloading conditions

\[
f \leq 0, \quad \dot{\lambda} \geq 0, \quad \dot{\lambda} f = 0 \quad \text{and} \quad \dot{\lambda} \dot{f} = 0
\]  

(100)

The determination of the analytical expressions for the Helmholtz free energy function \( \Psi \) and its identification from experiments is essential to the whole problem of modeling the plasticity phenomenon.
6 THERMODYNAMIC FORMULATION WITH HIGHER-ORDER GRADIENTS AND ANISOTROPIC HARDENING

An attempt is made to account for the effect of non-uniform distribution of micro-defects on the homogenized response of the material. This is done in order to be able to model small-scale phenomena, such as the effect of relative size on the mechanical properties of the material or the width of localization zones in softening media. The issue that necessitates resolution here is that classical plasticity theory as presented in the previous sections does not possess an intrinsic material length scale. This makes it incapable of predicting small-scale phenomena. However, by assuming that the internal energy depends not only on the internal state variables $\varepsilon^p$ and $p$, but also on its spatial higher-order gradients $\nabla \varepsilon^p$ and $\nabla p$, the aforementioned phenomena can be captured mathematically.

The third-order tensor $\left( \nabla \varepsilon^p \right)_{ijk} = \varepsilon_{ij,k}^p$ introduces kinematic hardening which is attributed to the net Burgers vector being not equal to zero at the microscale. The first-order gradient $\left( \nabla p \right)_k = p_{,k}$ introduces isotropic hardening or internal history which is attributed to the accumulation of the so-called geometrically necessary dislocations. The third order flux gradient tensor $\left( \nabla \alpha \right)_{ijk} = \alpha_{ij,k}$ introduces anisotropy through kinematic hardening as well as internal history. The plastic strain gradient, $\nabla \varepsilon^p$, is related to the geometrically necessary dislocation density tensor, $G$, through the following relation (Arsenlis and Parks, 1999):

$$ G_{ij} = e_{iq} \varepsilon_{jq,r}^p $$

(101)
where $e_{eq}$ is the permutation tensor. Additionally, the gradient of the effective plastic strain, $\nabla p$, can be related to the effective density of geometrically necessary dislocation, $\rho_G$, through the following relation (Ashby, 1970):

$$
\rho_G = \frac{\bar{r}}{b} \sqrt{p_k p_k}
$$

(102)

where $\bar{r}$ is the Nye factor introduced by Arsenlis and Parks (1999) to reflect the scalar measure of GND density resultant from macroscopic plastic strain gradients. For FCC polycrystals, Arsenlis and Parks (1999) reported a value of $\bar{r} = 1.85$ in bending and a value of $\bar{r} = 1.93$ in torsion for the Nye factor. Therefore, the presence of higher-order gradients through the plastic strain tensor (i.e. $\nabla \varepsilon$) leads to higher-order gradients in the accumulation of plastic strain (i.e. $\nabla p$) such that one cannot exist without the other.

Because of the presence of both $\nabla \varepsilon^\theta$ and $\nabla p$ the total rate of accumulation of the plastic strain gradients

$$
\dot{e} = \sqrt{\dot{p}^2 + \ell^2 \dot{p}_k \dot{p}_k}
$$

with

$$
e = \int_0^t \dot{e} \, dt
$$

(103)

should also be taken into account in the constitutive description since it introduces additional isotropic hardening. In obtaining the equality in Eq. (103), the gradient of the plastic strain direction, $\nabla N$, is neglected. This assumption is supported by the plastic deformation localization, whereby the plastic flow direction is almost the same within the localized zone. Moreover, adopting this assumption greatly simplifies the subsequent derivations. Hence, the generalized rate of total accumulation of the plastic strain and plastic strain gradients can be defined as (e.g. Fleck and Hutchinson, 2001; Gurtin, 2003; Gudmundson, 2004):
\[ \dot{E}^2 = \dot{\varepsilon}_0^p \dot{\varepsilon}_0^p + \ell^2 \dot{\varepsilon}_0^{p,k} \dot{\varepsilon}_0^{p,k} \] (104)

where \( \ell \) is the material length scale parameter and \( E = \int_0^t \dot{E} \, dt \) is the nonlocal effective plastic strain, intended to measure the total dislocation density. It must be noted that the physical justification of Eq. (104) is that \( E \) provides an overall scalar measure of the density of dislocations, with \( p \) giving a measure of statistically stored dislocation density and \( e \) providing a measure of the geometrically necessary dislocation density. If plastic strain gradients are absent, \( E \) can be reduced to the local effective plastic strain \( p \). It follows that for a complete constitutive description at small length scales, the internal power and the Helmholtz free energy should include not only the effects of \( p \) and \( \varepsilon \) but should also include the effects of \( \nabla \alpha \), \( \nabla p \), and \( e \). These variables may have a common origin in dislocation storage and motion, but they will be treated independent of each other. This gives different physical interpretations that lead to different evolution equations and allowing one the computational introduction of the influence of one scale on the other (e.g. mesoscale on macroscale). For example, dislocation interactions are observed on a mesolevel with length-scale \( 0.1-10 \mu m \) and strongly affect the material behavior on the macrolevel with length-scale \( \geq 100 \mu m \). In this model however, those variables are considered mathematically related to their local counterparts. Therefore, special care must be taken to properly account for their coupling.

It is important to note that some authors have considered in their thermodynamics formulation only the gradient of the plastic strain \( \nabla \varepsilon \) or the gradient of the kinematic flux \( \nabla \alpha \), while others have considered only the gradient of the effective plastic strain \( \nabla p \). But no one seems to have really considered the effect of both \( \nabla \alpha \) and \( \nabla p \) together.
For example, Fleck and Hutchinson (2001), Gao et al. (1999), Gurtin (2003, 2004), Gudmundson (2004) developed gradient theories that allow dependences on plastic strain gradients only. However, the theories of Fleck and Hutchinson and Gao introduce gradients in the plastic strain that only affect the isotropic hardening part with no kinematic hardening. Gurtin (2003, 2004) did not incorporate $\nabla p$ in his variational formulation, but was incorporated in the functional definition of the Helmholtz free energy. Aifantis (1984), Mühlhaus and Aifantis (1991), Acharya and Bassani (2000), Liebe and Steinmann (2001), and Polizzotto and Borino (1998) developed gradient theories that allow dependences on the accumulation of the plastic strain such that only the isotropic hardening part is affected by the presence of these gradients. Voyiadjis et al. (2001, 2003, 2004) introduced first and second order gradients in both isotropic and kinematic hardening. However, the kinematic hardening was introduced through an arbitrary flux variable. It must be emphasized that this model is developed on the conviction that both $\nabla \alpha$ and $\nabla p$ should enter the definitions of the internal virtual power and the Helmholtz free energy. Therefore, one can anticipate from the formulation in the previous sections that the conjugate force of $\nabla \alpha$ is the nonlocal back-stress while the conjugate force of $\nabla p$ is the nonlocal drag stress. This will be shown subsequently.

**Principle of Virtual Power**

It follows from the discussion above, that the dependence of the internal power on $\nabla \alpha$, $\nabla p$, and $e$ through the internal variable $E$ is the essential ingredient of the present strain gradient plasticity model. Therefore, the internal and external power expenditures are assumed to have the following forms, respectively,
\[
P_{\text{int}} = \int_{\Gamma} \left( \sigma_{ij} \dot{\epsilon}_{ij} + X_{ij} \dot{\gamma}_{ij} + R \dot{\gamma} + S_{ij} \dot{\gamma}_{j,\kappa} + Q_{\kappa} \dot{\gamma}_{j,\kappa} + K \dot{\gamma} \right) \, dV \tag{105}
\]
\[
P_{\text{ext}} = \int_{\Gamma} h_{ij} \gamma_{ij} \, dV + \int_{\partial \Gamma} t_{ij} \gamma_{ij} \, dA - \int_{\Gamma} \rho \dot{\gamma} \gamma_{ij} \, dV + \int_{\partial \Gamma} \left( m_{ij} \gamma_{ij} + q \dot{\gamma} \right) \, dA \tag{106}
\]

\(P_{\text{int}}\) and \(P_{\text{ext}}\) balance each other in the sense of Eq. (4). The kinematical fields in the expressions above are considered as virtual. Eq. (105) is based on the concept that the power expended by each kinematical field be expressible in terms of an associated force system consistent with its own balance (Gurtin, 2000). However, these kinematical fields are no longer independent. Therefore, special care is taken in the following sections to properly account for their coupling. The nature of this coupling can be determined using the principle of virtual power.

In Eq. (106) \(m\) is the microtraction tensor conjugate to \(\dot{\epsilon}^p\), defined for each unit vector \(n\) normal on the boundary \(\partial \Gamma\) of \(\Gamma\), and is symmetric and deviatoric since \(\dot{\epsilon}^p\) is symmetric and deviatoric. \(q\) is the microtraction force associated with the history variable \(\dot{\gamma}\). The force \(q\) is precisely that introduced by Fleck and Hutchinson (2001) in their representation of a variational principle governing the one-parameter theory, \(\nabla \gamma\).

The last integral term in Eq. (106) results in higher-order boundary conditions generally consistent with the framework of a gradient theory. The first three terms in Eq. (105) constitute the definition of the local internal virtual power as presented in Eq. (3). The last three terms in Eq. (105) are meant to take into account the large spatial variations in \(\epsilon^p\) at small length scales. The first of the last three terms represents the internal power generated by the nonlocal backstress \(S\) such that it introduces kinematic hardening through the net Burgers vector. The third-order tensor \(S\) also follows precisely that introduced by Gurtin (2000, 2002, 2003, 2004) in his thermodynamics of one-parameter
theory $\nabla \varepsilon''$. The last two terms in Eq. (105) represent the internal power generated by the nonlocal drag vector $Q$ and drag force $K$ which account for the additional isotropic hardening from the accumulation of geometrically necessary dislocations. As aforementioned, if the gradients in the plastic strain tensor are considered then the corresponding history variable $e$ defined in Eq. (103) must also be considered. The last term in Eq. (105), therefore, introduces the history in the accumulation of $\nabla \varepsilon''$ and $\nabla p$. This completes the consideration of the large variations in plasticity defects at the microscale.

Referring to the definition in Eq. (8) of the direction of the plastic strain, $N$, one can similarly define the directions of the plastic strain gradient, $\nabla \varepsilon''$, and the gradient of the effective plastic strain, $\nabla p$, respectively, as

$$
M_{ijk} = \frac{\varepsilon''_{ij,k}}{|\varepsilon''_{ij,k}|}, \quad N_{k} = \frac{\dot{p}_{k}}{|\dot{p}_{k}|} = \frac{\dot{p}_{k}}{\dot{\varepsilon}}
$$

(107)

where $M$ and $N$ define the unit tensors of $\nabla \varepsilon''$ and $\nabla p$, respectively, such that the $M : M = N : N = 1$. Therefore, it can easily be shown from Eqs. (107) that $N$, $M$, and $N$ are related by the following identity:

$$
N_{i}M_{jk}N_{k} = 1
$$

(108)

Moreover, from Eqs. (8) and (107) one can easily write

$$
\dot{p} = \dot{\varepsilon''}_{ij}N_{i}, \quad \dot{p}_{k} = \dot{\varepsilon''}_{ij,k}N_{i} \quad \dot{e} = \dot{\varepsilon''}_{ij,k}M_{ik}
$$

(109)

Utilizing Eq. (108) one can write Eq. (109) as

$$
\dot{e} = \dot{\varepsilon''}_{ij,k}N_{i}N_{k}
$$

(110)
Substituting the relation $\mathbf{\dot{e}}^e = \mathbf{\dot{e}} - \mathbf{\dot{e}}^p$ and Eqs. (109)$_1$, (109)$_2$, and (110) into Eq. (105) yields

$$P_{\text{int}} = \int \left\{ \sigma_{ij} \mathbf{\dot{e}}_{ij} - \left[ \tau_{ij} - kX_{ij} + (c\alpha_{mn}X_{mn} - R + cS_{mnk}\alpha_{mn,k})N_{ij} \right] \mathbf{\dot{e}}_{ij}^p \right\} \, dV$$

(Eq. 111)

Making use of Eq. (12) and applying the divergence theorem, Eq. (111) can be rewritten as follows:

$$P_{\text{int}} = -\int_{\Gamma} \sigma_{ij} \nu_i \, dV$$

$$-\int_{\Gamma} \left[ \tau_{ij} - kX_{ij} + kS_{ijk,k} - \left( R - c\alpha_{mn}X_{mn} + cS_{mnk}\alpha_{mn} - Q_k + KN_{k,k} \right)N_{ij} \right] \mathbf{\dot{e}}_{ij}^p \, dV$$

(Eq. 112)

Moreover, Eq. (106) can be rewritten by substituting Eq. (109)$_1$ as

$$P_{\text{ext}} = \int_{\Gamma} b_i \nu_i \, dV + \int_{\Gamma} t_i \nu_i \, dA - \int_{\Gamma} \rho \nu_i \nu_i \, dV + \int_{\Gamma} \mathbf{\dot{m}}_{ij} \mathbf{\dot{e}}_{ij}^p \, dA$$

(Eq. 113)

such that $\mathbf{\dot{m}} = \dot{k}\mathbf{m} + (q - c\mathbf{m} - \mathbf{a}) N$.

Applying the axiom of equilibrium of the principle of virtual power to the region $\Gamma$, Eq. (4), one obtains the following equilibrium equation

$$\int_{\Gamma} \left( t_i - \sigma_{ij} n_j \right) \nu_i \, dA + \int_{\Gamma} \left[ \mathbf{\dot{m}}_{ij} - \left( kS_{ijk} + (Q_k + KN_{k} - cS_{mnk})N_{ij} \right) n_k \right] \mathbf{\dot{e}}_{ij}^p \, dA$$

$$+ \int_{\Gamma} \left[ \tau_{ij} - kX_{ij} + kS_{ijk,k} - \left( R - Q_{k,k} - c\alpha_{mn}X_{mn} + cS_{mnk}\alpha_{mn} - KN_{k,k} \right)N_{ij} \right] \mathbf{\dot{e}}_{ij}^p \, dV = 0$$

(Eq. 114)

$\Gamma$, $\mathbf{v}$, and $\mathbf{\dot{e}}^p$ may be arbitrarily specified such that the classical macro-force balance and the macro-traction condition remain the same as presented, respectively, in Eqs. (14) and
while the micro-force balance condition undergoes a major change. Specifically, the micro-force balance takes the form

\[
\tau_{ij} - kX_{ij} + kS_{ijk,k} = - \left( R - Q_{k,k} - cX_{mn} \alpha_{mn} + cS_{mnk,k} \alpha_{mn} - KN_{k,k} - K_N N_k \right) N_{ij} = 0 \tag{microforce balance} \] (115)

which is supplemented by a micro-traction condition given by

\[
\tilde{m}_{ij} = \left[ kS_{ijk} + \left( Q_{k,k} - cX_{mn} \alpha_{mn} \right) N_{ij} \right] n_k \tag{microtraction condition} \] (116)

As concluded previously, the micro-force balance, Eq. (115), can be viewed as the plasticity yield condition. Thus, the micro-traction condition, Eq. (116), may be viewed as a higher-order condition (or internal boundary condition) augmented by the interaction of dislocations across interfaces (Gurtin, 2003; Gudmundsson, 2004). Moreover, it is noticed from Eq. (114) that since \( \dot{\varepsilon}^p \) is deviatoric, then \( \tilde{m} \) and \( \text{div}(S_{ijk}) = S_{ijk,k} \) are deviatoric while \( S \) is deviatoric in its first two arguments (i.e., \( S_{ik} = 0 \)).

**Nonlocal Yield Criterion**

Subsequently, it will be shown that the micro-force balance presented in Eq. (115) is nothing more than the nonlocal yield condition. Substituting Eq. (8) into Eq. (115), one can easily write the following expression for the flow rule in Eq. (9):4:

\[
N_{ij} = \frac{\tau_{ij} - kX_{ij} + kS_{ijk,k}}{R - Q_{k,k} - cX_{mn} \alpha_{mn} + cS_{mnk,k} \alpha_{mn} - KN_{k,k} - K_N N_k} \Rightarrow
\]

\[
\dot{\varepsilon}_{ij}^p = \frac{\tau_{ij} - X_{ij} + S_{ijk,k}}{R - Q_{k,k} - cX_{mn} \alpha_{mn} + cS_{mnk,k} \alpha_{mn} - KN_{k,k} - K_N N_k} \tag{117}
\]

Moreover, by taking the Euclidean norm \( \| \| \) of Eq. (115) one can also write

\[
\| \tau_{ij} - kX_{ij} + kS_{ijk,k} \| - \| R - Q_{k,k} - cX_{mn} \alpha_{mn} + cS_{mnk,k} \alpha_{mn} - KN_{k,k} - K_N N_k \| \| N_{ij} \| = 0 \tag{118}
\]

Since \( \| N_{ij} \| = 1 \) and
\[ \| R - Q_{k,k} - cX_{mn} \alpha_{mn} + cS_{mn,k} \alpha_{mn} - K N_{k,k} - K N_{k,k} \| = R - Q_{k,k} - cX_{mn} \alpha_{mn} + cS_{mn,k} \alpha_{mn} - K N_{k,k} - K N_{k,k} \]

one can then rewrite the above expression as

\[ \tau_{ij} - k X_{ij} + k S_{ijkl} \| - R + Q_{k,k} + cX_{mn} \alpha_{mn} - cS_{mn,k} \alpha_{mn} + K N_{k,k} + K N_{k,k} = 0 \]  \hspace{1cm} (119)

Therefore, micro-force balance, Eq. (115) can be set as the nonlocal yield criterion or the nonlocal plasticity loading surface \( f \)

\[ f = \| \tau_{ij} - k X_{ij} + k S_{ijkl} \| - R + Q_{k,k} + cX_{mn} \alpha_{mn} - cS_{mn,k} \alpha_{mn} + K N_{k,k} + K N_{k,k} = 0 \]  \hspace{1cm} (120)

such that the flow rule in Eq. (117)_2 can also be expressed by

\[ \dot{\varepsilon}_{ij}^p = \dot{p} \frac{\tau_{ij} - k X_{ij} + k S_{ijkl}}{\| \tau_{mn} - k X_{mn} + k S_{mn,k} \|} \]  \hspace{1cm} (121)

Comparing Eq. (121) with Eq. (8), one can rewrite the direction of the plastic flow as

\[ N_{ij} = \frac{\tau_{ij} - k X_{ij} + k S_{ijkl}}{\| \tau_{mn} - k X_{mn} + k S_{mn,k} \|} \]  \hspace{1cm} (122)

It may be noticed that higher-order stress \( \text{div} \{ S \} \) is a backstress quantity giving rise to kinematic hardening, while the stresses \( \text{div} \{ Q \} = Q_{k,k} \) and \( \text{div} \{ K N_{k,k} \} = K N_{k,k} + K N_{k,k} \) give rise to isotropic hardening. Furthermore, if the higher-order gradients are neglected, one can easily retrieve from Eqs. (120), (121), and (122), respectively, the classical yield criterion, Eq. (72), flow rule, Eq. (73), and flow direction, Eq. (74).

**Nonlocal Clausius-Duhem Inequality**

Utilizing the derived micro-force balance, Eq. (115), and the micro-traction condition, Eq. (116), into Eq. (112), the expression for the internal power defined in Eq. (105) can be rewritten as follows:

\[ P_{in} = \int_R \sigma_{ij} \dot{\varepsilon}_{ij} dV + \int_{\partial T} \tilde{m}_{ij} \dot{\varepsilon}_{ij}^p dA \]  \hspace{1cm} (123)
Comparing the above equation with its corresponding local expression, Eq. (23), implies that the nonlocal energy interactions can be non-vanishing only within the plastic zone. Hence, the energy term \( \int_{\partial \Omega} \tilde{m}_{ij} \dot{\epsilon}_{ij} dA \) may be described as the nonlocality energy residual that results from microstructural interactions between the material points in the active plastic zone (Eringen and Edelen, 1972). Similar arguments have been presented by Polizzotto and Borino (1998). They assumed \( \int_{\partial \Omega} \tilde{m}_{ij} \dot{\epsilon}_{ij} dA = 0 \) and described it as the insulation condition, implying that nonlocal energy is not allowed to flow from any point in \( \Gamma \) to the exterior of the body. However, their arguments were based on physical justifications rather than mathematically derived.

Furthermore, Eq. (123) coincides with the classical definition in Eq. (23) if the micro-traction term \( \int_{\partial \Omega} \tilde{m}_{ij} \dot{\epsilon}_{ij} dA \) is set to zero. This yields the standard definition of the internal power presented in Eq. (23) and postulated by Green and Naghdi (1971), which has also been used by numerous researchers over the last three decades. Therefore, the application of the following internal micro-boundary conditions on the plastic interfaces may be required

\[
\tilde{m}_{ij} \dot{\epsilon}_{ij} = 0 \quad \text{on} \quad \partial \Gamma^p \quad \text{(124)}
\]

where \( \partial \Gamma^p \subseteq \partial \Gamma \) is the plastic boundary. The above equation gives two different conditions according to a split of the plastic subdomain boundary into external and internal parts such that \( \partial \Gamma^p = \partial \Gamma^p_{\text{int}} \cup \partial \Gamma^p_{\text{ext}} \) (Polizzotto and Borino, 1998). Thereby one boundary condition is imposed on the external plastic boundary \( \partial \Gamma^p_{\text{ext}} \subseteq \partial \Gamma \)

\[
\tilde{m}_j = 0 \quad \text{on} \quad \partial \Gamma^p_{\text{ext}} \quad \text{(125)}
\]
which corresponds to the so-called Neumann type boundary. This *microtraction-free* boundary condition is the simplest form of Eq. (116) and assumes that the moment tractions $\mathbf{m}$ vanish at the external surfaces $\partial\Gamma_{\text{ext}} = \partial\Gamma^p \cap \partial\Gamma$ (i.e. unmovable external surfaces). Moreover, Eq. (125) places no constraint on the plastic flow and could characterize free dislocation movements across the boundaries. If external surface tractions exist, the macro-traction $t$ in Eq. (15) has a value whereas the micro-traction $\mathbf{m}$ vanishes.

The other condition is imposed on the internal plastic boundary $\partial\Gamma_{\text{int}}$ such that

$$\hat{\dot{\epsilon}}_{ij}^p = \mathbf{0} \text{ on } \partial\Gamma_{\text{int}}$$

(126)

which corresponds to a continuity boundary condition of Dirichlet type. This condition arises from the consideration that, in general, the stress rate $\mathbf{\dot{\sigma}}$ is continuous across $\partial\Gamma_{\text{int}}$. Therefore, the related elastic strain rate, $\dot{\epsilon}^e$, and plastic strain rate, $\dot{\epsilon}^p$, must be continuous. Moreover, this *microplastic-clamped* boundary condition places a constraint on the plastic flow and could characterize the dislocation blocking at the interface. Meanwhile, $\partial\Gamma_{\text{int}}$ characterizes the movable elastic-plastic boundary.

However, $\mathbf{m}$ is meant to be the driving force at the material internal boundaries such that generally $\mathbf{m} \neq \mathbf{0}$. Hence, for an intermediate (i.e. not free and not clamped) kind of boundary condition (i.e. $\mathbf{m} \neq \mathbf{0}$ on $\partial\Gamma_{\text{ext}}$ and $\hat{\dot{\epsilon}}_{ij}^p \neq \mathbf{0}$ on $\partial\Gamma_{\text{int}}$), one can define the density of the nonlocality energy residual, $\mathbb{R}$, as follows

$$\int_{\Gamma} \mathbb{R} \, dV = \int_{\partial\Gamma} \mathbf{m}_j \hat{\dot{\epsilon}}_{ij}^p \, dA$$

(127)

Therefore, if one neglects the interior surface energy that results from dislocation interactions at the internal boundaries (e.g. internal boundaries at inclusions), the
insulation condition of Polizzotto (e.g. Polizzotto and Borino, 1998; Polizzotto, 2003) can
be expressed as
\[
\int_{\Gamma} \mathbb{R} \, dV = 0 \tag{128}
\]
By substituting the expression for \( \mathbf{m} \) from Eq. (116) into Eq. (127) and applying the
divergence theorem, one obtains
\[
\int_{\Gamma} \mathbb{R} \, dV = \int_{\Gamma} \left( \left[ kS_{ijk} + (Q_k + KN_k - cS_{mnk} \alpha_{mn}) N_{ij} \right] \dot{\varepsilon}_{ij}^p \right) \, dV \tag{129}
\]
As mentioned previously, the consideration here is a purely mechanical theory (i.e.
processes are isothermal) based on the requirement that the rate of change in the total free
energy should be less than or equal to the power done by external forces (Gurtin, 2000).
Consequently, by substituting Eqs. (123) and (127) into Eq. (26), the following
thermodynamic restriction is obtained in a point wise form:
\[
\sigma_{ij} \dot{\varepsilon}_{ij} - \rho \dot{\Psi} + \mathbb{R} \geq 0 \tag{130}
\]
where \( \mathbb{R} \) is given by
\[
\mathbb{R} = \left( \left[ kS_{ijk} + (Q_k + KN_k - cS_{mnk} \alpha_{mn}) N_{ij} \right] \dot{\varepsilon}_{ij}^p \right)_{k}
= \left[ kS_{ijk,k} + (Q_{k,k} + KN_{k,k} + K_{k}N_{k,k} - cS_{mnk,k} \alpha_{mn,k} - cS_{mnk,k} \alpha_{mn}) N_{ij} \right] \dot{\varepsilon}_{ij}^p
+ \left[ kS_{ijk} + (Q_k + KN_k - cS_{mnk} \alpha_{mn}) N_{ij} \right] \dot{\varepsilon}_{ij,k}^p \tag{131}
\]
The inequality in Eq. (130) may be described as the nonlocal Clausius-Duhem
inequality. This differs from its classical counterpart, Eq. (27), only because of the
presence of the nonlocality residual \( \mathbb{R} \). This inequality holds everywhere in \( \Gamma \), but
\( \mathbb{R} = 0 \) at material points in the elastic zone. Moreover, it can be obtained from Eq. (131)
that for a homogeneous strain distribution \( \mathbb{R} = 0 \) and one retains the classical Clausius-
Duhem inequality.

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Next the nonlocal Clausius-Duhem inequality in Eq. (130) will be employed for deriving the thermodynamic restrictions upon the inherent constitutive equations, to be satisfied for any admissible deformation mechanism.

**Nonlocal State Variables**

Now it is possible to continue considering constitutive equations of the form presented in Section 2.3, but with the higher-order gradients, $\nabla \alpha$, $\nabla p$, and $e$ added to the list of internal state variables. Specifically, the definition of the state $\hat{\mathbf{N}}_k (k = 1, ..., n_m)$ in Eq. (81) can be generalized to include the nonlocal internal variables from the internal power expression, Eq. (105), such that

$$\hat{\mathbf{N}}_k = \mathbf{\hat{N}}_k \left( \alpha_{ij}, p, \alpha_{ij,k}, p_k, e \right)$$

(132)

Therefore, it is part of this model’s philosophy that the nonlocal variables $\nabla \alpha$, $\nabla p$, and $e$ must appear in the specific free energy $\Psi$ since they contribute to the internal power expression.

Assuming a separable material, the Helmholtz free energy potential can be written as

$$\Psi = \Psi^e \left( \varepsilon_{ij}^e \right) + \Psi^p \left( \alpha_{ij}, p, \alpha_{ij,k}, p_k, e \right)$$

(133)

Taking the time derivative of Eq. (133) with respect to its internal state variables yields

$$\dot{\Psi} = \frac{\partial \Psi^e}{\partial \varepsilon_{ij}^e} \dot{\varepsilon}_{ij}^e + \frac{\partial \Psi^p}{\partial \alpha_{ij}} \dot{\alpha}_{ij} + \frac{\partial \Psi^p}{\partial p} \dot{p} + \frac{\partial \Psi^p}{\partial \alpha_{ij,k}} \dot{\alpha}_{ij,k} + \frac{\partial \Psi^p}{\partial p_k} \dot{p}_k + \frac{\partial \Psi^p}{\partial e} \dot{e}$$

(134)

Making use of Eqs. (109) and (110) in Eq. (134), yields

$$\dot{\Psi} = \frac{\partial \Psi^e}{\partial \varepsilon_{ij}^e} \dot{\varepsilon}_{ij}^e + \left[ k \frac{\partial \Psi^p}{\partial \alpha_{ij}} \dot{\alpha}_{ij} + \left( \frac{\partial \Psi^p}{\partial p} - c \frac{\partial \Psi^p}{\partial \alpha_{mn}} \alpha_{mn} - c \frac{\partial \Psi^p}{\partial \alpha_{mn,k}} \alpha_{mn,k} \right) N_{ij} \right] \dot{\varepsilon}_{ij}^p$$

$$+ \left[ k \frac{\partial \Psi^p}{\partial \alpha_{ij,k}} + \left( \frac{\partial \Psi^p}{\partial p_k} - \frac{\partial \Psi^p}{\partial e} N_{ij} - c \frac{\partial \Psi^p}{\partial \alpha_{mn,k}} \alpha_{mn} \right) N_{ij} \right] \dot{\varepsilon}_{ij,k}^p$$

(135)
The nonlocal Clausius-Duhem inequality from Eq. (130) can now be applied to the present case along the expanded time derivative in Eq. (135) such that

\[
\left(\sigma_{ij} - \rho \frac{\partial \Psi^e}{\partial \epsilon_{ij}^e}\right) \dot{\epsilon}_{ij}^e
\]

\[+ \left(\tau_{ij} - \rho k \frac{\partial \Psi^p}{\partial \alpha_{ij}} - \rho \left(\frac{\partial \Psi_p}{\partial p} - c \frac{\partial \Psi_p}{\partial \alpha_{mm}} \alpha_{mn} - c \frac{\partial \Psi_p}{\partial \alpha_{mm,k}} \alpha_{mn,k}\right) N_{ij}\right) \dot{\epsilon}_{ij}^p
\]

\[= \rho k \frac{\partial \Psi^p}{\partial \alpha_{ij,k}} + \rho \left(\frac{\partial \Psi_p}{\partial p_k} + \frac{\partial \Psi_p}{\partial \epsilon} \mathbf{N}_k - c \frac{\partial \Psi_p}{\partial \alpha_{mn,k}} \alpha_{mn}\right) N_{ij} \dot{\epsilon}_{ij,k}^p + \mathbb{R} \geq 0
\]

(136)

A classical hypothesis permits the canceling of the first term in this inequality. Independently from the inequality the thermodynamic laws in Eqs. (85) and (86) are obtained along with the following nonlocal thermodynamic state law

\[
\mathbb{Z}_{ijk} = \rho k \frac{\partial \Psi^p}{\partial \alpha_{ij,k}} + \rho \left(\frac{\partial \Psi_p}{\partial p_k} + \frac{\partial \Psi_p}{\partial \epsilon} \mathbf{N}_k - c \frac{\partial \Psi_p}{\partial \alpha_{mn,k}} \alpha_{mn}\right) N_{ij}
\]

(137)

From Eqs. (136), (86), and (137), one can rewrite the nonlocal Clausius-Duhem inequality in Eq. (136) as

\[
\Pi = J_{ij} \dot{\epsilon}_{ij}^p - \mathbb{Z}_{ijk} \dot{\epsilon}_{ij,k}^p + \mathbb{R} \geq 0
\]

(138)

where \(\Pi\) is the nonlocal dissipation energy per unit volume.

**Nonlocal Plastic Flow Rule**

By making use of the Onsager reciprocity principle (Malvern, 1969), which is assumed to hold also in the case of nonlocal material behavior, the specific dissipation energy in Eq. (138) can be expressed in a linear form in terms of the driving flux, \(\dot{\epsilon}^p\), and related thermodynamic force, similar to the expression in Eq. (87), such that

\[
\Pi = \tilde{J}_{ij} \dot{\epsilon}_{ij}^p \geq 0
\]

(139)
where \( \mathbf{J} \) denotes the unknown total quasi-nonlocal thermodynamic force. By comparing Eqs. (138) and (139), the nonlocality residual \( R \) can be expressed by

\[
R = \begin{bmatrix} \mathbf{J}^p_{ij} \varepsilon^p_{ij} - \mathbf{J}^p_{ij} \varepsilon^p_{ij} + \mathbb{Z}_{ijk} \varepsilon^p_{ij,k} 
\end{bmatrix}
\]  

(140)

On imposing the insulation condition in Eq. (128) with setting \( \Gamma = \Gamma^p \) such that \( \Gamma^p \subseteq \Gamma \) is the region of \( \Gamma \) where the plastic deformation is taking place, one can write from Eq. (140)

\[
\int_{\Gamma^p} \left[ \begin{bmatrix} \mathbf{J}^p_{ij} \varepsilon^p_{ij} - \mathbf{J}^p_{ij} \varepsilon^p_{ij} + \mathbb{Z}_{ijk} \varepsilon^p_{ij,k} \end{bmatrix} dV = 0 \right.
\]  

(141)

Upon applying the divergence theorem to the last term in Eq. (141), one can write

\[
\int_{\Gamma^p} \left( \begin{bmatrix} \mathbf{J}^p_{ij} - \mathbf{J}^p_{ij} - \mathbb{Z}_{ijk} \varepsilon^p_{ij,k} \end{bmatrix} \varepsilon^p_{ij} dV + \int_{\partial\Gamma^p} \mathbb{Z}_{ijk} n_k \varepsilon^p_{ij} dA = 0 \right.
\]  

(142)

Since Eq. (142) must hold for any plastic deformation mechanism, and for any possible evolution law as well; hence, for any arbitrary choice of \( \varepsilon^p \) in \( \Gamma^p \cup \partial\Gamma^p \), the necessary and sufficient conditions prove to be the following:

\[
\tilde{\mathbf{J}}_{ij} = \mathbf{J}^p_{ij} + \mathbb{Z}_{ijk} \varepsilon^p_{ij,k} \quad \text{in } \Gamma^p
\]  

(143)

and

\[
\mathbb{Z}_{ijk} n_k \varepsilon^p_{ij} = 0 \quad \text{on } \partial\Gamma^p
\]  

(144)

It is obvious that Eq. (143), after substitution of Eqs. (86) and (137), identifies the total quasi-nonlocal thermodynamic force \( \mathbf{J} \) in \( \Gamma^p \) and, therefore, it is the force that must be introduced into the evolution equations as the pertinent hardening/softening driving force. \( \mathbf{J} \) is a quasi-nonlocal force since it is decomposed into a local part, \( \mathbf{J}^p \), and a nonlocal part, \( \operatorname{div}(\mathbb{Z}) \). Eq. (144) provides the nonstandard boundary conditions.

Substitution of Eq. (143) into Eq. (140) gives
\[ R = Z_{ijk,k} \dot{\varepsilon}^p_{ij} + Z_{ijk} \dot{\varepsilon}^p_{ij,k} = \left( Z_{ijk} \dot{\varepsilon}^p_{ij} \right)_k \]  \hspace{1cm} (145)

such that \( R \neq 0 \) in \( \Gamma^p \), but \( R = 0 \) out of \( \Gamma^p \) or for a homogeneous plastic deformation.

Now substituting Eq. (137) into Eq. (145) and comparing the result with Eq. (131) yields the following expressions for the nonlocal thermodynamic conjugate forces

\[ S_{ijk} = \rho \frac{\partial \Psi}{\partial \alpha_{ij,k}} , \quad Q_k = \rho \frac{\partial \Psi}{\partial p_{j,k}} , \quad K = \rho \frac{\partial \Psi}{\partial e} \]  \hspace{1cm} (146)

Hence, one can rewrite \( Z \) in Eq. (137), after substituting Eqs. (146), as

\[ Z_{ijk} = kS_{ijk} + \left( Q_k + KN_k - cS_{mnk} \alpha_{mn} \right) N_{ij} \]  \hspace{1cm} (147)

Moreover, substituting Eq. (147) into Eq. (144) yields the same micro-traction boundary condition derived from the principle of virtual power, Eq. (116) or (124), such that the corresponding thermodynamic conjugate force is

\[ \tilde{m}_j = Z_{ijk} n_k \]  \hspace{1cm} (148)

which in turn yields the same non-standard boundary conditions presented in Eqs. (125) and (126).

Substitution of Eq. (143) into Eq. (139) yields the following expression for \( \Pi \)

\[ \Pi = \left( J_{ij} + Z_{ijk,k} \right) \dot{\varepsilon}^p_{ij} \geq 0 \]  \hspace{1cm} (149)

That is, \( R \) has disappeared from \( \Pi \) in Eq. (138), but its nonlocality has been replaced by \( \text{div} (Z) \). Substituting the expression for \( \dot{\varepsilon}^p \) from Eq. (9) into Eq. (149) and defining

\[ \gamma = \left( J_{ij} + Z_{ijk,k} \right) N_{ij} \geq 0 \]  \hspace{1cm} (150)

yields Eq. (37) (i.e. \( \Pi = \gamma \mu \geq 0 \)), where \( \gamma \) is interpreted here as the nonlocal dissipation modulus. Furthermore, equating Eqs. (37) and (149) gives Eqs. (38) and (39), but with \( \tilde{J} \) is given by Eq. (143) instead of Eq. (86), such that the plastic flow direction \( N \) is expressed
as
\[
N_{ij} = \frac{\tilde{J}_{ij} - J_{ij} + Z_{ijk,k}}{\|J_{mn} - J_{mn} + Z_{mnk,k}\|} \quad (151)
\]

By substituting Eqs. (86) and (147) into the above expression, Eq. (151) can be rewritten as
\[
N_{ij} = \frac{\tau_{ij} - \rho k \frac{\partial \Psi}{\partial \alpha_{ij}} + k S_{ijk,k}}{\gamma + \rho \frac{\partial \Psi}{\partial p} - Q_{k,k} - (K N_{k})_k} \quad (152)
\]

Comparing Eqs. (152) and (122), one can write
\[
\tilde{J}_{ij} = \tau_{ij} - k X_{ij} + k S_{ijk,k} \Rightarrow \|\tilde{J}_{ij} - k X_{ij} + k S_{ijk,k}\| = R - Q_{k,k} - (K N_{k})_k \quad (153)
\]
such that the back-stress \(X\) and the micro-force \(R\) are given by Eqs. (94) and (95), respectively. Therefore, one can express the nonlocal plastic flow rule as presented previously in Eq. (121) with the thermodynamic conjugate forces \(\sigma, X, S, R, Q, K\) as given by Eqs. (85), (94), (95), (146)\(_1\), (146)\(_2\), (146)\(_3\), respectively. Thus, the essential change in the classical plasticity theory is that here the size of the yield surface depends on the gradient of the effective plastic strain \(\nabla \varepsilon^p\) and effective plastic strain gradient \(e\); while the center of the yield surface depends on the kinematic flux gradient \(\nabla \alpha\).

**Nonlocal Evolution Equations**

Equation (139), which holds with Eqs. (125) and (126), expresses the plastic dissipation density, \(\Pi\), through the local evolution of \(\dot{\varepsilon}^p\) and the related thermodynamic force \(\tilde{J}\). Therefore, in case of associative plasticity, as is the case here, a consistent way to establish the plastic evolution laws is by making use of the maximum plastic dissipation principle introduced in Section 2.5. This can be also used to find the evolution
equations of the nonlocal internal variables $\nabla \alpha$, $\nabla p$, and $e$. Therefore, substituting Eq. (139) into Eq. (96) and applying the calculus of several variables, one can write

$$\frac{\partial \Omega}{\partial J_{ij}} = 0 \Rightarrow \frac{\partial \Omega}{\partial \sigma_{ij}} = 0, \quad \frac{\partial \Omega}{\partial X_{ij}} = 0, \quad \frac{\partial \Omega}{\partial S_{ijk,k}} = 0$$

(154)

$$\frac{\partial \Omega}{\partial R} = 0, \quad \frac{\partial \Omega}{\partial Q_{k,k}} = 0, \quad \frac{\partial \Omega}{\partial (KN_k)_k} = 0$$

(155)

and

$$\frac{\partial \Omega}{\partial S_{ijk}} = 0, \quad \frac{\partial \Omega}{\partial Q_{k}} = 0, \quad \frac{\partial \Omega}{\partial K} = 0$$

(156)

By making use of Eqs. (86), (143), and (137) along with Eqs. (94), (95), and (146) the plastic flow rule, $\dot{\varepsilon}^p$, can then be obtained from any of the conditions in Eq. (154), such that

$$\dot{\varepsilon}^p_{ij} = \dot{\lambda} \frac{\partial f}{\partial J_{ij}} \Rightarrow \dot{\varepsilon}^p_{ij} = \dot{\lambda} \frac{\partial f}{\partial \sigma_{ij}} = \frac{\dot{\lambda}}{k} \frac{\partial f}{\partial X_{ij}} = \frac{\dot{\lambda}}{k} \frac{\partial f}{\partial S_{ijk,k}}$$

(157)

which agrees with the classical assumption that the plastic flow direction $N$ is governed by the Cauchy stress $\sigma$. However, Eq. (157) suggests that similarly $N$ is governed by the nonlocal microstress $\text{div}(S)$, such that

$$N_{ij} = \frac{\partial f}{\partial \sigma_{ij}} = -\frac{\partial f}{\partial X_{ij}} = \frac{\partial f}{\partial S_{ijk,k}}$$

(158)

or equivalently $N$ can be expressed by Eqs. (117) or (122). The evolution of $\dot{p}$ can be obtained from any of the conditions in Eq. (155) along with Eq. (120) such that

$$\dot{p} = -\dot{\lambda} \frac{\partial f}{\partial R} = \dot{\lambda} \frac{\partial f}{\partial Q_{k,k}} = \dot{\lambda} \frac{\partial f}{\partial (KN_k)_k} = \dot{\lambda}$$

(159)
where $\hat{\lambda}$ is the plastic multiplier which can be determined by the nonlocal consistency condition similar to that in Eq. (99). Moreover, the expressions in Eqs. (157) and (158) agree well with the previously derived expressions, namely those in Eqs. (121) and (122).

By substituting Eq. (159) into Eq. (109)$_2$, one can write the flow rule of plastic strain gradient as
\[
\dot{\varepsilon}^{p}_{ij,k} = \hat{\lambda}_{,k}N_{ij}
\]  
(160)
such that $\nabla \hat{\rho} = \nabla \hat{\lambda}$, while the evolution equation of $\dot{\varepsilon}$ can be obtained from Eqs. (107)$_2$ and (120) such that
\[
\dot{\varepsilon} = \hat{\lambda}_{,k}N_{k}
\]  
with
\[
N_{k} = \frac{\partial f}{\partial K_{,k}}
\]  
(161)
Moreover, one can rewrite an evolution law for $\nabla \varepsilon^{p}$, other than Eq. (160), from Eq. (107)$_1$ as
\[
\dot{\varepsilon}^{p}_{ij,k} = \dot{\varepsilon}M_{ijk} \quad \text{with} \quad M_{ijk} = N_{ij}N_{k} = \frac{\partial f}{\partial S_{ij,m}} \frac{\partial f}{\partial K_{,k}}
\]  
(162)
The three conditions in Eq. (156) give, respectively,
\[
\frac{\partial f}{\partial S_{jk}} = 0, \quad \frac{\partial f}{\partial Q_{k}} = 0, \quad \frac{\partial f}{\partial K} = 0
\]  
(163)
which does not agree with the proposition of Gurtin (2000, 2003) and Gudmundson (2004) who argued that the plastic flow direction $\mathbf{N}$ is governed by the microstress $\mathbf{S}$ and not the Cauchy stress $\mathbf{\sigma}$. However, in this model the classical assumption is reiterated that $\mathbf{N}$ is governed by $\mathbf{\sigma}$ or equivalently by the microstress, $\text{div}(\mathbf{S})$. 

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Gradient-Dependence of the Helmholtz Free Energy

In order to develop equations amenable to the analysis and computation, some consideration is given to the definition of the Helmholtz free energy function.

One can assume decoupling between the elastic behavior and plasticity hardening (i.e. separable material) such that both $\Psi^e$ and $\Psi^p$ that appear in Eq. (133) can be assumed to have the following quadratic analytical form:

$$\rho \Psi^e = \frac{1}{2} \varepsilon^e_{ij} E_{ijkl} \varepsilon^e_{kl}$$

(164)

$$\rho \Psi^p = \frac{1}{2} a_i \varepsilon^p_{ij} \varepsilon^p_{ij} + \frac{1}{2} a_2 p^2 + \frac{1}{2} a_2 \alpha_j \alpha_j + \frac{1}{2} a_5 p_{.k} p_{.k} + \frac{1}{2} a_6 e^2 + \frac{1}{2} a_6 \alpha_{.k} \alpha_{.k}$$

(165)

where $E$ is the symmetric fourth-order elastic stiffness tensor and $a_i$ ($i=1-5$) are material constants. However, utilizing the following relations

$$p^2 = \varepsilon^p_{ij} \varepsilon^p_{ij} , \quad e^2 = \varepsilon^p_{ij} \varepsilon^p_{ij} = p_{.k} p_{.k}$$

(166)

respectively, from Eqs. (60) and (103), one can equivalently write Eq. (165) as

$$\rho \Psi^p = \frac{1}{2} \left( a_1 + a_2 \right) p^2 + \frac{1}{2} \left( a_3 + a_4 + a_5 \right) e^2$$

(167)

Moreover, by assuming that the hardening moduli $h = a_1 + a_2$ and $h \ell^2 = a_3 + a_4 + a_5$, one can rewrite Eq. (167) as

$$\rho \Psi^p = \frac{1}{2} h \left( p^2 + \ell^2 e^2 \right) = \frac{1}{2} h E^2$$

(168)

where the generalized effective plastic strain $E$ is given by Eq. (104).

Now, one can obtain the Cauchy stress from Eqs. (85) and (164) such that

$$\sigma_{ij} = E_{ijkl} \varepsilon^e_{kl} = E_{ijkl} \left( \varepsilon^e_{kl} - \varepsilon^p_{kl} \right)$$

(169)
and the local and nonlocal conjugate forces by making use of Eqs. (94), (95), (146), respectively, as follows:

\[ X_{ij} = h\alpha_{ij} \]  

\[ R = \gamma + hp \]  

\[ S_{ijk} = h\ell^2 \varepsilon_{ijk}^p \]  

\[ Q_k = h\ell^2 p_k \]  

\[ K = h\ell^2 e \]

where \( \gamma \) coincides with the initial coarse-grain yield strength for rate and temperature independent materials. Moreover, substituting Eqs. (172)-(174) into the yield function \( f \), Eq. (120), one can then write

\[ f = \|\mathbf{r}_{ij} - X_{ij} + S_{ijk,k}\| - \gamma - h\left[ p - \ell^2 \left( \nabla^2 p + \|\nabla_i p\|\nabla_{k,k} + e_k\nabla_{k,k} \right) \right] = 0 \]  

with

\[ S_{ijk,k} = h\ell^2 \nabla^2 \varepsilon_{ij}^p \]  

where \( \nabla^2 \) designates the Laplacian operator and \( \nabla_{k,k} \) designates the first gradient vector.

For monotonic and proportional loading (in the case of isotropic hardening) one can easily show by using Eqs. (103) and (107)\( _2 \) that the last two terms in the left-hand-side of Eq. (175) can be reduced to

\[ \|\nabla_i p\|\nabla_{k,k} + e_k\nabla_{k,k} = \nabla^2 p \]  

such that \( f \) can be given by

\[ f = \|\mathbf{r}_{ij} - X_{ij} + S_{ijk,k}\| - \gamma - hp + 2h\ell^2\nabla^2 p = 0 \]
Thus this theory shows that the Laplacian of the effective plastic strain contributes to the size of the yield surface (isotropic hardening) and the Laplacian of the plastic strain contributes to the movement of the center of the yield surface (kinematic hardening). It is also noteworthy that the present formulation links hardening to the gradients of plastic strain $\nabla \varepsilon^p$ and the effective plastic strain $\nabla p$ and, respectively, not to $\nabla^2 \varepsilon^p$ and $\nabla^2 p$, consistent with basic notions of the role of the net Burgers vector and the geometrically necessary dislocations. Instead, $\nabla^2 \varepsilon$ and $\nabla^2 p$ emerges in the resulting field equations as a byproduct of the more fundamental role of the plastic strain gradients.

The next sections present some applications of the gradient plasticity model. Of particular interest is the model’s ability to describe size effects observed in metals. The proposed gradient plasticity theory is used to investigate the size dependent behavior in biaxial loading of a plastic thin film on an elastic substrate and shear loading of a thin film fixed to a rigid substrate. In the following applications the expression of the yield surface $f$ in Eq. (178) is employed.

**Biaxial Loading of a Thin Film on a Substrate**

A biaxially loaded isotropic elasto-plastic thin film of thickness $T$ on a thick semi-infinite elastic substrate is considered as shown in Figure 3. Let $x_3$ be the perpendicular axis to the film with $x_3 = 0$ corresponding to the film-substrate interface. The loading is defined by a monotonically increasing biaxial strain $\varepsilon_o$ such that $\varepsilon_{11} = \varepsilon_{22} = \varepsilon_o$. 
A plane stress situation is assumed such that the non-vanishing stress components are

\[ \sigma_{11} = \sigma_{22} = \sigma_o(x_3) \]  

(179)

From the plastic incompressibility assumption and the symmetry, one can write the non-vanishing plastic strain components as

\[ \varepsilon_{11}^p = \varepsilon_{22}^p = -\frac{1}{2} \varepsilon_{33}^p = \varepsilon_o^p(x_3) \]  

(180)

Therefore the total and plastic strain tensors may be written in matrix format as

\[
\varepsilon = \begin{bmatrix}
\varepsilon_0(x_3) & 0 & 0 \\
0 & \varepsilon_0(x_3) & 0 \\
0 & 0 & 0
\end{bmatrix}
\quad \text{and} \quad
\varepsilon^p = \begin{bmatrix}
\varepsilon_0^p(x_3) & 0 & 0 \\
0 & \varepsilon_0^p(x_3) & 0 \\
0 & 0 & -2\varepsilon_0^p(x_3)
\end{bmatrix}
\]  

(181)

Meanwhile, using the conditions of plastic incompressibility and symmetry, the plane and deviatoric stress tensors may be written in matrix format as
Finally, the kinematic flux and deviatoric part of the microstress (backstress) may be written in matrix format as

\[
\alpha_{ij} = \begin{bmatrix} \alpha_{11}(x_3) & 0 & 0 \\ 0 & \alpha_{22}(x_3) & 0 \\ 0 & 0 & \alpha_{33}(x_3) \end{bmatrix} \quad \text{and} \quad X_{ij} = \begin{bmatrix} X_{11}(x_3) & 0 & 0 \\ 0 & X_{22}(x_3) & 0 \\ 0 & 0 & X_{33}(x_3) \end{bmatrix}
\]  

(183)  

The effective plastic strain \( p = \sqrt{\varepsilon^p_{ij} \varepsilon^p_{ij}} \) and its Laplacian \( \nabla^2 p \) are given as

\[
p = \sqrt{6\varepsilon^p_{ij} \varepsilon^p_{ij}} \quad \text{and} \quad \nabla^2 p = \sqrt{6\varepsilon^p_{ij} \varepsilon^p_{ij}}
\]  

(184)  

where \( \varepsilon^p_{ij} = \frac{\partial \varepsilon^p}{\partial x_i} \left( \frac{\partial \varepsilon^p}{\partial x_j} \right) \).

The stress-strain relationship can be obtained from the generalized Hooke’s law as

\[
\sigma_0(x_3) = \frac{E}{(1-\nu)} \left( \varepsilon_0 - \varepsilon^p_0(x_3) \right)
\]  

(185)  

Substituting Eqs. (179), (184), and (185) into the yield condition, Eq. (178), yields the implicit differential equation below:
It is obvious that a closed-form solution is not feasible for such a complex equation. A numerical approximation method must therefore be used to obtain results. However, even a numerical solution requires additional parameters to be established before an approximation method may be executed.

It is worthwhile to note that $\dot{\alpha}$ and $\dot{\varepsilon}_0^p$ are related by Equation (52). For monotonic loading, and at any given point $i$ along $x_3$, the kinematic flux may be related to the plastic strain by solving Equation (52) as a differential equation. This yields the following relations

$$\alpha_{11}(i) = \alpha_{22}(i) = \sqrt{6k \cosh(i)} \left(1 - e^{-\phi_x}\right)$$

$$\alpha_{33}(i) = \sqrt{6k \cosh(i)} \left(-2 - e^{-\phi_x}\right)$$  \hspace{1cm} (187)

Use of these expressions requires discretization of Equation (186) along $x_3$.

Discretizing Equation (186), substituting Equations (187) into the resulting expression, and using the Central Finite Difference Method, yields a set of $n$ equations, where $n$ represents the number of points along $x_3$ in the mesh. However, the Central Finite
Difference Method produces \( n+2 \) unknowns, where two of the unknowns represent the fictional plastic strain at the “virtual” points outside the physical bounds of the thin film. This is where the boundary conditions at either edge of the film come in.

The micro-boundary conditions can be utilized as presented by Eqs. (125) and (126). The microtraction-free boundary condition is imposed at the free surface (i.e. \( x_3 = t \)) and the microplastic-clamped boundary condition is imposed at the film-substrate interface such that \( \frac{\partial \bar{\varepsilon}^p_o}{\partial z} = 0 \) at \( z = 1 \) and \( \bar{\varepsilon}^p_o = 0 \) at \( z = 0 \) \hspace{1cm} (188)

The \( n \) equations from the Finite Difference formulation, along with these micro-boundary condition expressions are solved using the computer mathematics package Mathcad.

![Figure 4: Biaxial Plastic Strain through the Film Thickness](image)

Figure 4: Biaxial Plastic Strain through the Film Thickness
The stress along the film can be found by using the plastic strain results with Eq. (185).

Furthermore the average stress in the thin-film, $\bar{\sigma}_o$, can be determined from an integration of $\sigma$ from 0 to 1.

Figure 5: Biaxial Stress through the Film Thickness

Figure 6: Average Biaxial Strain versus Biaxial Strain
Results in Figure 4, 5, and 6 are presented for $h(1-\nu)/E=0.05$ and $\nu=0.3$. Different film thicknesses are represented by $\ell/t=0.1, 0.5, 1, 1.5, 2$. In Figure 6, normalized results for average film stress versus applied biaxial strain $\varepsilon_p$ are presented. It is clearly seen that the hardening tangent modulus increases with decreasing the film thickness, which agrees qualitatively with the experimental observations. Figures 4 and 5 show the variation of the biaxial stress and plastic strain across the film thickness. Instead of a uniform distribution of stress and plastic strain across the film thickness, according to classical local plasticity, the stress increases and the plastic strain decreases as the film-substrate interface is approached. Moreover, the results clearly show that the biaxial stress and plastic strain profiles tend to become homogeneous with increased thickness due to smaller gradient effects. This means that gradients eventually disappear for large thicknesses. As shown in Figure 4, the increase of plastic strain at $x_3=t$ overwhelms the increase as the substrate is approached due to the distribution of gradients, which is lower as the free boundary is approached and higher at the substrate. The elimination of gradients spreads from the free boundary, propagating through the entire thickness. Finally, the plastic strain becomes uniform across the thickness.

**Shear Loading of a Thin Film on a Substrate**

An elasto-plastic thin film is bonded to a rigid substrate under pure shear loading as shown in Figure 7. Thereafter, the bottom surface of the film is held fixed and a shear traction is applied to the top surface in the $x_1$-direction. The film is assumed to be infinitely long in the $x_1$-direction and initially homogeneous and, therefore, the solution depends only on $x_3$. 

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Shu et al. (2001) simulated this problem in a discrete dislocation calculation of constrained plastic flow within a crystalline layer. The only non-vanishing stress and plastic strain components are

\[ \sigma_{31} = \tau_o, \quad \varepsilon_{31}^p = \frac{1}{2} \gamma_0^p(x_3) \]  

(189)

where \( \tau_o \) is homogeneous across the film thickness since the macroscopic force balance, Eq. (66), yields \( \partial \tau_o / \partial x_3 = 0 \) if body forces and inertia are neglected.

According to these assumptions the total and plastic strain tensors may be written in matrix format as

\[
\varepsilon_{ij} = \begin{bmatrix}
0 & 0 & \gamma_0(x_3) \\
0 & 0 & 0 \\
\gamma_0(x_3) & 0 & 0
\end{bmatrix}
\quad \text{and} \quad
\varepsilon_{ij}^p = \begin{bmatrix}
0 & 0 & \gamma_0^p(x_3) \\
0 & 0 & 0 \\
\gamma_0^p(x_3) & 0 & 0
\end{bmatrix}
\]  

(190)

Meanwhile, using the conditions of plastic incompressibility and symmetry, the plane and deviatoric stress tensors are identical and may be written in matrix format as
\[
\sigma_{ij} = \begin{bmatrix} 0 & 0 & \tau_0(x_3) \\ 0 & 0 & 0 \\ \tau_0(x_3) & 0 & 0 \end{bmatrix} \text{ and } \tau_{ij} = \begin{bmatrix} 0 & 0 & \tau_0(x_3) \\ 0 & 0 & 0 \\ \tau_0(x_3) & 0 & 0 \end{bmatrix}
\]

(191)

Finally, the kinematic flux and deviatoric part of the microstress (backstress) may be written in matrix format as

\[
\alpha_{ij} = \begin{bmatrix} 0 & 0 & \alpha_0(x_3) \\ 0 & 0 & 0 \\ \alpha_0(x_3) & 0 & 0 \end{bmatrix} \text{ and } X_{ij} = \begin{bmatrix} 0 & 0 & X_0(x_3) \\ 0 & 0 & 0 \\ X_0(x_3) & 0 & 0 \end{bmatrix}
\]

(192)

The effective plastic strain \( p = \sqrt{e_{ij}^p e_{ij}^p} \) and its Laplacian \( \nabla^2 p \) are given as

\[
p = \frac{\sqrt{2}}{2} \gamma_o^p (x_3) \text{ and } \nabla^2 p = \frac{\sqrt{2}}{2} \gamma_{o,33}^p
\]

(193)

where \( \gamma_{o,33}^p = \frac{\partial \gamma_o^p}{\partial x_3} \frac{\partial \gamma_o^p}{\partial x_3} \). The stress-strain relationship is given by Hooke’s law as

\[
\tau_o = G \left( \gamma_o - \gamma_o^p (x_3) \right)
\]

(194)

where \( G \) is the elastic shear modulus. Substituting Eqs. (189) and (193) into the yield condition, Eq. (178), yields the implicit differential equation below:

\[
\begin{aligned}
2G^2 (\gamma_0 - \gamma_o^p)^2 - ka_3 G \alpha_0 (\gamma_0 - \gamma_o^p) + 4kh^2 l^2 G \alpha_0 (\gamma_0 - \gamma_o^p) + 2k^2 a_3 \alpha_0^2 & -4a_3 kh^2 l^2 \alpha_0 \alpha_0^{\dddot} + 2h^2 k^2 l^4 (\alpha_0^{\dddot})^2 \\
& \left[ \frac{1}{2} \frac{\gamma}{m} - \frac{\sqrt{2}}{2} \frac{h}{m} \gamma_o^p + \frac{\sqrt{2}}{2} hl^2 \gamma_o^{\dddot} \\
& - \frac{1+m}{m} 2ca_3 \alpha_0^2 - 2chl^2 \alpha_0 \alpha_0^{\dddot} + \sqrt{2} hl^2 \alpha_0^{\dddot} \right] = 0
\end{aligned}
\]

(195)

The same methodology is used as for the biaxial case with the following relation

\[
\alpha_0(i) = \frac{\sqrt{2} k}{2c} \left( 1 - e^{-\frac{\sqrt{2}}{2} \gamma_o^{p}(i)} \right)
\]

(196)
The microtraction-free boundary condition is imposed at $x_3 = t$ and the microplastic-clamped boundary condition is imposed at $x_3 = 0$ such that one can write, respectively, the following

$$\frac{\partial \tau_o^p}{\partial z} = 0 \text{ at } z = 1 \quad \text{and} \quad \tau_o^p = 0 \text{ at } z = 0 \quad (197)$$

The n equations from the Finite Difference formulation, along with these micro-boundary condition expressions are solved using the computer mathematics package Mathcad.

![Figure 8: Plastic Shear Strain across the Film Thickness](image)

The stress along the film can be found by using the plastic strain results with Eq (194).
Results in Figures 8 and 9 are presented for $h/G=0.15$. Different film thicknesses are captured by different $\ell/t$. Similar results to biaxial loading are obtained. Figure 8 shows the variation of the plastic shear strain, across the film thickness that corresponds to an applied strain $\gamma_0 = 4\gamma_y$. Instead of a uniform distribution across the film thickness, the plastic shear strain decreases as the fixed surface is approached. For a thick film, equivalent to $\ell/t \rightarrow 0$, the results would coincide with the local plasticity theory solution, which would give homogeneous plastic strain in the film. If $\ell/t \rightarrow \infty$ a pure elastic state would be obtained in the film. It is also noted from Figure 9 that the maximum $\gamma_o^p$ in the film is determined by the local theory solution. Hence, for a gradient-dependent behavior, the plastic shear at the top of the film can either equal or fall below the local limit, depending on the thickness of the film. Moreover, noticeable departures from the classical limit are seen in Figure 9 for the material length scale as small as $\ell/t=0.1$. 
Comparison with Gudmundson’s Model

The model by Gudmundson (Gudmundson, 2004) is considered the standard-bearer for strain gradient applications in thin films. Gudmundson’s model included the gradient terms used here, however it used plastic strain as the conjugate variable to backstress. The result for his closed form solution for the biaxial case is presented below:

![Figure 10: Biaxial Strain through Film Thickness for Gudmundson’s Model](image)

The results from Gudmunson’s model are comparable to the results from the current model, with two noticeable differences. First, the current model exhibits a greater “boundary layer”. That is, the gradient hardening effects propagate further into the thickness of the film then they do for Gudmundson’s model. Secondly, though not entirely unrelated, the current model exhibits a strengthening effect. This means that as the length scale to thickness ratio becomes greater, the average stress rises more dramatically in the current model. This can be better seen when the stress along the film thickness is plotted.
Meanwhile, the results for the shear problem from Gudmundson’s model are presented below:

Figure 11: Biaxial Stress through Film Thickness for Gudmundson’s Model

Figure 12: Shear Strain through Film Thickness for Gudmundson’s Model
Similar effects are seen for the shear problem as for the biaxial problem. The current model has a greater boundary layer than Gudmundson’s, and the strengthening is more pronounced.

![Figure 13: Shear Stress through Film Thickness for Gudmundson’s Model](image)

The figure below illustrates the strengthening by plotting average stress vs. the length to thickness ratio for the biaxial loading case.

![Figure 14: Average Biaxial Stress versus Normalized Length Scale](image)
8 CONCLUSIONS

- In this work a thermodynamic framework is proposed that extends the classical formulation of the plasticity theory to higher-order gradient plasticity theory and has the potential to cover a wide range of strain gradient plasticity effects. Higher-order stresses and higher-order boundary conditions are formulated in a consistent way. A nonlocal form of the Clasusius-Duhem inequality is formulated based on the virtual power principle where only the primary variables and their first-order gradients enter the variational formulation.

- The proposed theory is a three nonlocal parameter theory that takes into account large variations in the plastic strain, large variations in the accumulated plastic strain, and accumulation of plastic strain gradients. Both isotropic and kinematic gradient-hardening effects are considered.

- An effort has been made to reveal the higher-order nature of the gradient-dependent theory as clearly as possible. The existence of the higher-order stresses requires some change to the conventional interpretation of the field equations. The formulation of higher-order boundary conditions is very important within strain gradient plasticity theory, especially, at the interfaces, grain, or phase boundaries. If these boundary conditions are not considered in solving the size effect problem and without assuming the existence of initial heterogeneity, the solution would be homogeneous with no gradients. Therefore, strain gradients come into play if the boundaries are assumed to constrain the plastic flow. Hence, this is a central part of the further development of strain gradient plasticity theory.
Illustrations are given in this paper for both constrained and unconstrained plastic deformation at a boundary by employing a simplified form of the constitutive equations. In the present examples of a thin film-substrate system, the substrate is assumed to be rigid, or elastic but stiff, where dislocations in the film are blocked as they approach the boundaries. A continuum model of this situation must require the plastic strain to vanish at such a boundary. By contrast, dislocations approaching a free surface are free to pass out and producing unconstrained plastic strain at the surface. Micro- traction boundary conditions of this situation must require the plastic strain gradients to vanish at such a boundary.

Applications of the model to thin films on elastic substrates for biaxial and shear loading conditions are investigated. The effect of relative size (length scale) is exhibited in the numerical computations.

The model captures increased hardening as the length scale is approached. This is similar to other strain gradient models. Unlike other models, however, this model also captures strengthening of the material as the length scale is approached. This demonstrates the usefulness and

In conclusion, if continuum theories are to be used to predict elastic–plastic behavior at the micron or sub-micron length scales, a higher-order theory is the best all-around approach..
REFERENCES


APPENDIX: MATHCAD FILE

Values of Constants c and k

Find values for k and c in the expression for kinematic flux: \[
\frac{d\alpha}{dt} = k \cdot \frac{d\varepsilon_p}{dt} - c \cdot \frac{d\varepsilon_p}{dt} \cdot \alpha
\]

For monotonic loading, we can write the following expression:
\[
\alpha(\varepsilon_p) = \left(\frac{\sqrt{6}}{6c}\right) \left(k - k e^{-\sqrt{6}c\varepsilon_p}\right)
\]

Expression for kinematic flux from Voyiajs and Abu Al Rub (2003)
\[
A(\varepsilon_p) := \frac{3}{2} \cdot \left[ -\frac{1}{300000} \cdot \left(1 - e^{-\frac{11765\pi}{300000}}\right) + \frac{1}{300000} \cdot \left(1 - e^{-\frac{5882\pi}{300000}}\right) + \frac{67}{80000} \cdot \left(1 - e^{-\frac{940\pi}{80000}}\right) + \frac{33}{17300} \cdot \left(1 - e^{\frac{-411\pi}{17300}}\right) \right]
\]

The two expressions are not equivalent, but we can solve for k and c if we assume they have equal values at two values of plastic strain. We are interested in values of strain up to 1%. Therefore it makes sense to choose k and c such that our kinematic flux is most similar to the FAPC model at points in this range. Values of strain of 0.4% and 1% seem appropriate as they capture the range.

"Seed" values: \(k := 1\), \(\delta_\alpha = 100\)

Given
\[
\left(\frac{\sqrt{6}}{6c}\right) \cdot \left(k - k e^{-\sqrt{6}c0.004}\right) = A(0.004)
\]
\[
\left(\frac{\sqrt{6}}{6c}\right) \cdot \left(k - k e^{-\sqrt{6}c0.01}\right) = A(0.01)
\]

\((k, c) := \text{Find}(k, c)\)

Solution Values
\(k = 2.173\)
\(c = 208.053\)

\[
\alpha(\varepsilon_p) := \left(\frac{\sqrt{6}}{6c}\right) \left(k - k e^{-\sqrt{6}c\varepsilon_p}\right)
\]

![Graph showing values of \(\alpha(\varepsilon_p)\) and \(A(\varepsilon_p)\) over \(\varepsilon_p\) values.]

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Vita

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