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A thermodynamic based higher-order gradient theory for size dependent plasticity

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Abstract

A physically motivated and thermodynamically consistent formulation of small strain higher-order gradient plasticity theory is presented. Based on dislocation mechanics interpretations, gradients of variables associated with kinematic and isotropic hardenings are introduced. This framework is a two non-local parameter framework that takes into consideration large variations in the plastic strain tensor and large variations in the plasticity history variable; the equivalent (effective) plastic strain. The presence of plastic strain gradients is motivated by the evolution of dislocation density tensor that results from non-vanishing net Burgers vector and, hence, incorporating additional kinematic hardening (anisotropy) effects through lattice incompatibility. The presence of gradients in the effective (scalar) plastic strain is motivated by the accumulation of geometrically necessary dislocations and, hence, incorporating additional isotropic hardening effects (i.e. strengthening). It is demonstrated that the non-local yield condition, flow rule, and non-zero microscopic boundary conditions can be derived directly from the principle of virtual power. It is also shown that the local Clausius–Duhem inequality does not hold for gradient-dependent material and, therefore, a non-local form should be adopted. The non-local Clausius–Duhem inequality has an additional term that results from microstructural long-range energy interchanges between the material points within the body. A detailed discussion on the physics and the application of proper microscopic boundary conditions, either on free surfaces, clamped surfaces, or intermediate constrained surfaces, is presented. It is shown that there is a close connection between interface/surface energy of an interface or free surface and the microscopic boundary conditions in terms of microtraction stresses. Some generalities and utility of this theory are discussed and comparisons with other gradient theories are given. Applications of the proposed theory for size effects in thin films are presented.

Keywords: Gradient plasticity; Non-local; Size effect; Thin films

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1. Introduction

The problem in developing a macroscopic model embedded with a micromechanical-based theory of plasticity which could be used as an engineering theory for both the analysis and in computer-aided design of materials is a topical and still unsolved problem. Attempts to construct such a theory are faced with the difficulties in describing the microscopic structure of materials in terms of macroscopic mechanics. On the other hand, at the present time, it is still not possible to perform quantum and atomistic simulations on realistic time scale and structures. When load is applied, the inelastic deformation that occurs in most cases is not homogeneous, but reveals fluctuations on various length scales. This heterogeneity plays a key role in determining the macroscopic properties of materials. A theory that bridges the gap between the conventional continuum theories and the micromechanical theories should be developed as a remedy for this situation.

The emerging areas of micro and nanotechnologies exhibit important strength differences that result from continuous modification of the material microstructural characteristics with changing size, whereby the smaller is the size the higher is the strength of the material. There are many experimental observations which indicate that, under certain specific conditions, the specimen size may significantly affect deformation and failure of the engineering materials and a length scale is required for their interpretation. For example, experimental work on particle-reinforced composites has revealed that a substantial increase in the macroscopic flow stress can be achieved by decreasing the particle size while keeping the volume fraction constant (Lloyd, 1994; Rhee et al., 1994; Zhu and Zbib, 1995; Nan and Clarke, 1996; Kiser et al., 1996). A similar strengthening effect associated with decreasing the diameter of thin wires in micro-torsion test has been reported by Fleck et al. (1994) and with decreasing the thickness of thin beams in micro-bending test has been reported by Stolken and Evans (1998), Shrotriya et al. (2003), and Haque and Saif (2003). Moreover, micro- and nano-indentation tests have shown that the material hardness increases with decreasing indentation size (e.g. Stelmashenko et al., 1993; DeGuzman et al., 1993; Ma and Clarke, 1995; Poole et al., 1996; McElhaney et al., 1998; Lim and Chaudhri, 1999; Elmustafa and Stone, 2002; Swadener et al., 2002). The experimental work by Taylor et al. (2002) shows an increase in the flow stress with decreasing hole size for geometrically similar perforated plates under tension.

The aforementioned dependence of mechanical response on size could not be explained by the classical continuum mechanics since no length scale enters the constitutive description. A multiscale continuum theory, therefore, is needed to bridge the gap between the classical continuum theories and micromechanical theories. In all of the problems mentioned above, a continuum approach is appropriate since the collective nature of material defects is sufficiently large and faraway from individuality. Moreover, since the increase in strength with decreasing scale can be related to proportional increase in the strain gradients in each of the aforementioned experiments, the gradient plasticity theory has been successful in addressing the size effect problem. This success stems out from the incorporation of a microstructural length scale parameter through functional dependencies on the plastic strain gradient of non-local media (Aifantis, 1984, 1987). The gradient-dependent theory abandons the assumption that the stress at a given point is uniquely determined by the history of strain at this point only. It takes into account possible interactions with other material points in the vicinity of that point. However, in the past decade, the physical basis of the gradient plasticity theory for metals has been founded on theoretical developments concerning geometrically necessary dislocations (GNDs). Standard micromechanical modeling of the inelastic material behavior of metallic single crystals and polycrystals is commonly based on the premise that resistance to glide is due mainly to the random trapping of mobile dislocations during locally homogeneous deformation. Such trapped dislocations are commonly referred to as statistically stored dislocations (SSDs), and act as obstacles to further dislocation motion, resulting in hardening. As anticipated in the work of Ashby (1970) an additional contribution to the density of immobile dislocations and so to hardening can arise when the continuum length scale approaches that of the dominant microstructural features. An extensive review of the recent developments in gradient-dependent theory can be found in Abu Al-Rub (2004). A short review of these developments is presented here.

Many researchers have contributed substantially to the gradient approach with emphasis on numerical aspects of the theory and its implementation in finite element codes (e.g. Lasry and Belytschko, 1988; Zbib and Aifantis, 1988; de Borst and Mühlhaus, 1992; de Borst et al., 1993; Pamin, 1994; de Borst and Pamin, 1996; Bammann et al., 1999; Abu Al-Rub and Voyiadjis, 2005; Voyiadjis and Abu Al-Rub, in press). In par-

allel, other approaches that have length scale parameters in their constitutive structure (commonly referred to as non-local integral theories) have appeared as an outgrowth of earlier work by Eringen in non-local continuum elasticity and phenomenological hardening plasticity (e.g. Eringen and Edelen, 1972) and Bazant in strain softening media (e.g. Pijaudier-Cabot and Bazant, 1987; Bazant and Pijaudier-Cobot, 1988). Another class of gradient theories have been advocated in the last decade that assume higher-order gradients of the displacement field (e.g. Fleck et al., 1994; Fleck and Hutchinson, 1993, 1997, 2001; Nix and Gao, 1998; Gao et al., 1999; Gao and Huang, 2001; Hwang et al., 2002; Gurtin, 2000, 2003). This group of theories is in fact a particular case of the generalized continua, such as *micromorphic continua* (Eringen, 1968), or *continua with microstructure* (Mindlin, 1964), which were all inspired by the pioneering work of the Cosserat brothers (Cosserat and Cosserat, 1909). The *Cosserat continuum* (or *micropolar continuum*) enhances the kinematic description of deformation by an additional field of local rotations, which can depend on the rotations corresponding to the displacement field, i.e. on the skew-symmetric part of the displacement gradient for the small displacement theory, or on the rotational part of the polar decomposition in the large-displacement theory. However, the works of Mindlin, Cosserat, and Eringen are based on the classical balances of linear and angular momentum. In contrast, the works of Fleck and Gurtin involve the introduction of additional balances over and above these classical balances; e.g. for single-crystal plasticity there is a new balance for each slip system involving forces that expend power in consort with slip on that system. Dislocation based gradient plasticity theories that are motivated by the generation of GNDs and incompatibility of lattice deformation have been advanced by Acharya and Bassani (2000), Acharya and Beaudoin (2000), Bassani (2001), Voyiadjis and Abu Al-Rub (2004, 2005), and Abu Al-Rub and Voyiadjis (2006, in press). However, these theories preserve the same structure of classical plasticity with no additional boundary conditions.

Numerous variational formulations and thermodynamic frameworks have also been proposed since the 1990s in order to extend the classical (local) constitutive theory to a non-local (gradient-dependent) theory. However, these constitutive models are far from being firmly established. Moreover, the various proposals are also quite different with respect to the structure of the equations. Mühlhaus and Aifantis (1991) formulated the classical (local) incremental variational principle by incorporating first-order gradients of the effective (scalar) plastic strain variable which contributes to the isotropic hardening/softening plasticity. Extra boundary conditions and higher-order stresses were derived. However, in their formulation the higher-order tractions that result from higher-order gradients were not considered. Fleck and Hutchinson (2001) reformulated their earlier theory (Fleck and Hutchinson, 1993, 1997) based on the variational principle of Mühlhaus and Aifantis (1991) but with different constitutive structure. In the formulation of Fleck and Hutchinson (2001) higher-order tractions, higher-order stresses, and extra boundary conditions were derived. Valanis (1996) and Fremond and Nedjar (1996) postulated the dependence of the Helmholtz free energy on scalar variables and on its first-order gradients. Additionally, they checked the consistency of their constitutive equations using the classical (local) form of the Clausius–Duhem inequality. However, Polizzotto (e.g. Polizzotto and Borino, 1998; Polizzotto, 2003) assumed a non-local form of the Clausius–Duhem inequality based on the concept of non-locality energy residual introduced by Eringen and Edelen (1972). First- and second-order gradients of the effective plastic strain were incorporated in their formulation in which the non-locality residual enters the definition of the Clausius–Duhem inequality as an extra term that accounts for the energy exchanges between the particles in the domain of interest at the microstructural level. Moreover, Polizzotto proposed the insulation condition, which assumes the vanishing of the total non-local residuals over the whole volume of the body, in order to derive the extra boundary conditions. The thermodynamic framework of Polizzotto was used by Steinmann (e.g. Mentzel and Steinmann, 2000; Liebe and Steinmann, 2001) to derive several strain gradient plasticity models where the second-order gradient of the effective plastic strain was incorporated. Shizawa and Zbib (1999) derived a rigorous thermodynamical theory of finite strain gradient plasticity by incorporating kinematic gradient hardening effects through the concept of dislocation density tensor. Similar gradient-based thermodynamic framework was proposed by Svendsen (2002). Another thermodynamic approach was developed by Gurtin (e.g. Gurtin, 2000, 2002, 2003, 2004) who treated the plastic strain gradients as independent variables, which is different than the above frameworks, and introduced the concept of microforce balance, which is shown in this paper to be equivalent to the yield condition. Gurtin introduced both isotropic and kinematic gradient hardening effects and argued that the plastic flow direction is governed by a microstress, obtained from the microforce balance, and not the deviatoric Cauchy stress. In Gurtin's

framework, however, only kinematic hardening variables enter the variational formulation without the isotropic hardening variables. Very similar framework has been proposed by Gudmundson (2004). Bammann (2001) has developed a dislocation based thermodynamic framework that incorporates the effect of geometrically necessary dislocations through the curl of the plastic deformation gradient. Thermodynamic approaches to gradient-dependent plasticity and damage models were developed by Voyiadjis and co-workers (Voyiadjis et al., 2001, 2003, 2004; Abu Al-Rub and Voyiadjis, 2006, in press) who postulated the dependence of the Helmholtz free energy on scalar and tensorial hardening/softening variables and its second-order gradients. However, no explicit treatment of non-standard boundary conditions was considered in this framework. Clayton et al. (2006) presented a novel finite deformation thermodynamic framework to describe spatial rotational gradients in crystals by introducing a mathematical concept for geometrically necessary disclinations at grain boundaries. However, the effects of these rotational gradients are expected to be minimal in small strain problems.

The gradient theory has been applied to interpret size-dependent phenomena including, shear banding, micro- and nano-indentation, twist of thin wires, bending of thin films, void growth, crack tip plasticity, fine-grained metals, strengthening in metal matrix composites, multilayers, etc. (see Abu Al-Rub (2004) for a detailed review). Therefore, practical applications of gradient-dependent theories include, but not limited to, sensors, actuators, microelecromechanical systems (MEMS), microelectronic packaging, advanced composites, micromachining, welds, and functionally graded materials. However, the full utility of the gradient-type theories in bridging the gap between modeling, simulation, and design of modern technology hinges on one's ability to determine accurate values for the constitutive length scale parameter that scales the effects of strain gradients. The study of Begley and Hutchinson (1998), Nix and Gao (1998), Shu and Fleck (1998), Yuan and Chen (2001), Abu Al-Rub and Voyiadjis (2004a,b), and Abu Al-Rub (2004) indicated that indentation experiments might be the most effective test for measuring the length scale parameter ℓ. Moreover, in spite of the crucial importance of the length scale parameter in gradient theory, very limited work is focused on the physical origin of this length scale parameter. The discrete dislocation origin of this length scale is rarely clear and its value is a free parameter. However, initial attempts have been made to relate ℓ to the microstructure of the material. Nix and Gao (1998) identified ℓ as L^2/b, where L is the average spacing between dislocations, and b is the magnitude of the Burgers vector. Moreover, Abu Al-Rub and Voyiadjis (2004a,b), and Voyiadjis and Abu Al-Rub (2004) found ℓ to be proportional to the mean free path of the dislocations, L. Abu Al-Rub and Voyiadjis (2004b) also derived an evolution equation for ℓ as a function of temperature, strain, strain-rate, and a set of measurable microstructural physical parameters. Voyiadjis and Abu Al-Rub (2005) and Abu Al-Rub and Voyiadjis (2006, in press) found that the length scale varies with the course of plastic deformation, grain size, characteristic dimension of the specimen, and hardening exponent.

The objective of this paper is to develop a consistent thermodynamic framework that extends the J_2 flow theory to include the effects of strain gradients. This is achieved within the extent of small strain/small rotation plasticity and rate-independent material response. The pioneering works contributed by, among others, Aifantis, Eringen, Gurtin, Polizzotto, Fleck, and Hutchinson, and their co-workers, have been the source of inspiration to this work. The concepts of non-locality residual, the principle of virtual power, the second-law of thermodynamics, the maximum dissipation theorem, and the Onsager reciprocity principle are used in this paper to extend the well-known procedures of classical thermodynamics and local-type constitutive theory to gradient-dependent theory. This theory is a two non-local parameter theory that takes into account large variations in the plastic strain tensor and large variations in the accumulated (scalar) plastic strain. Both isotropic and kinematic gradient hardening effects are considered in the present work. In addition, a framework for the formulation of consistent microscopic boundary conditions is presented. It is shown in this work that there is a close connection between the microtraction stress and the surface/interface energy density of an interface or free surface as proposed by Fredriksson and Gudmundson (2005). Using a simplified version of the proposed theory, the length scale effects are investigated in detail for biaxial tension, pure shear, and temperature decrease for a thin film on a thick substrate.

The layout of this paper is as follows: In Section 2, crystallographic evidence for the presence of strain gradients is presented based on non-vanishing Burgers vector and the accumulation of geometrically necessary dislocations. In Section 3, the gradient plasticity theory is formulated based on the principle of virtual power and the second-law of thermodynamics. Section 4 presents some examples for the functional dependence of

the Helmholtz free energy on strain gradients. Section 5 presents some recent applications of gradient plasticity to handle size effects in metallic thin films.

1.1. Notation

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

2. Crystallographic basis for presence of plastic strain gradients

2.1. Basic kinematics

The classical theory of isotropic plastic solids undergoing small deformations is based on the additive decomposition of the displacement gradient, $\nabla\mathbf{u}$, into elastic and plastic parts, where $\nabla\mathbf{u}^{\mathrm{e}}$ being the elastic component and $\nabla\mathbf{u}^{\mathrm{p}}$ being the corresponding plastic component such that:

$$u_{i,j} = u^{\mathrm{e}}_{i,j} + u^{\mathrm{p}}_{i,j}, \quad u^{\mathrm{p}}_{k,k} = 0 \tag{1}$$

where the superscripts 'e' and 'p' designate the elastic and plastic components, respectively. The component $\nabla\mathbf{u}^{\mathrm{e}}$ represents rotation and stretching of the material structure, while the component $\nabla\mathbf{u}^{\mathrm{p}}$ represents the plastic distortion and characterizes the evolution of dislocations and other defects through this structure.

For small-strain formulation in classical continuum theory, the total second-order strain tensor, $\boldsymbol{\varepsilon}$, is defined by the symmetric part of the displacement gradient $\nabla\mathbf{u}$ such that

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

which can also be decomposed into elastic and plastic parts, where $\boldsymbol{\varepsilon}^{\mathrm{e}}$ being the elastic component and $\boldsymbol{\varepsilon}^{\mathrm{p}}$ being the corresponding plastic component such that:

$$\varepsilon_{ij} = \varepsilon^{\mathrm{e}}_{ij} + \varepsilon^{\mathrm{p}}_{ij}, \quad \varepsilon^{\mathrm{p}}_{kk} = 0 \tag{3}$$

The components $\boldsymbol{\varepsilon}^{\mathrm{e}}$ and $\boldsymbol{\varepsilon}^{\mathrm{p}}$ are the symmetric parts of $\nabla\mathbf{u}^{\mathrm{e}}$ and $\nabla\mathbf{u}^{\mathrm{p}}$, respectively, and are given by

$$\varepsilon^{\mathrm{e}}_{ij} = \frac{1}{2}(u^{\mathrm{e}}_{i,j} + u^{\mathrm{e}}_{j,i}), \quad \varepsilon^{\mathrm{p}}_{ij} = \frac{1}{2}(u^{\mathrm{p}}_{i,j} + u^{\mathrm{p}}_{j,i}) \tag{4}$$

From the kinematics of dislocation motion, the plastic part of the displacement gradient arising solely from slips, $p^{(\beta)}$, on all systems ($\beta = 1, \ldots, N$) is taken to be

$$u^{\mathrm{p}}_{i,j} = \sum_{\beta} p^{(\beta)} s^{(\beta)}_i n^{(\beta)}_j \tag{5}$$

where $\mathbf{s}^{(\beta)}$ and $\mathbf{n}^{(\beta)}$ are the unit vectors characterizing the slip direction on the slip plane β and its normal, respectively, such that $\|\mathbf{s}^{(\beta)}\| = \|\mathbf{n}^{(\beta)}\| = 1$ and $\mathbf{s}^{(\beta)} \cdot \mathbf{n}^{(\beta)} = 0$.

Substituting Eq. (5) into Eq. $(4)_2$ gives the plastic strain tensor in terms of the plastic slip as

$$\varepsilon^{\mathrm{p}}_{i,j} = \sum_{\beta} p^{(\beta)} \mu^{(\beta)}_{ij} \tag{6}$$

where $\boldsymbol{\mu}^{(\beta)}$ is the symmetric Schmidt orientation tensor given by

$$\mu^{(\beta)}_{ij} = \frac{1}{2}(s^{(\beta)}_i n^{(\beta)}_j + n^{(\beta)}_i s^{(\beta)}_j) \tag{7}$$

2.2. Nye's dislocation density tensor and geometrically necessary dislocations

Material deformation in metals enhances the dislocation formation, the dislocation motion, and the dislocation storage. The dislocation storage causes material hardening. The stored dislocations generated by trapping each other in a random way are referred to as statistically stored dislocations (SSDs), while the stored dislocations that maintain the plastic deformation compatibilities (continuity) within the polycrystal (or various components of the material) caused by non-uniform dislocation slip are called geometrically necessary dislocations (GNDs). Their presence causes additional storage of defects and increases the deformation resistance by acting as obstacles to the SSDs (Nye, 1953; Kröner, 1962; Ashby, 1970).

In order to account for strain-gradient effects, one makes use of the GNDs concept. The Nye's dislocation density tensor $\boldsymbol{\alpha}$, which is a representation of GNDs such that α_{ij} is the i-component of the resultant Burgers vector related to GNDs of line vector j, is defined as (Nye, 1953; Fleck and Hutchinson, 1997; Arsenlis and Parks, 1999; Bassani, 2001)

$$\alpha_{ij} = \sum_{\xi} \rho_G^{(\xi)} b_i^{(\xi)} t_j^{(\xi)} \tag{8}$$

where $\rho_G^{(\xi)}$ is the density of GNDs along slip system $\xi = 1, \ldots, G$, $\mathbf{b}^{(\xi)}$ is the Burgers vector, and $\mathbf{t}^{(\xi)}$ is the unit vector tangent to a GND. It can be noticed that SSDs do not contribute to the Nye's tensor. Moreover, the distribution of SSDs is redundant such that it can be assumed to be uniformly distributed over the crystal, while the distribution of GNDs is non-redundant and is non-uniform.

The total accumulation of GNDs is obtained as the magnitude of Nye's dislocation density tensor such that

$$\alpha = \sqrt{\alpha_{ij}\alpha_{ij}} = \sqrt{\sum_{\xi} \sum_{\zeta} H^{(\xi,\zeta)} \rho_G^{(\xi)} \rho_G^{(\zeta)} b_i^{(\xi)} b_i^{(\zeta)} t_j^{(\xi)} t_j^{(\zeta)}} \tag{9}$$

where $H^{(\xi,\zeta)} = H^{(\zeta,\xi)} (H^{(\zeta,\zeta)} = 1)$ is a dimensionless matrix which phenomenologically attempts to account for the interaction among different slip systems (resulting in the so-called *latent hardening*). However, for the sake of simplicity, one can neglect the interaction among different slip systems (i.e. $H^{(\xi,\zeta)} = \delta_{\xi\zeta}$, $\delta_{\xi\zeta}$, being the Kronecker delta), in which case α reads as follows:

$$\alpha = b\rho_G \tag{10}$$

where $b = \sqrt{\mathbf{b}^{(\xi)} \cdot \mathbf{b}^{(\xi)}}$ is the magnitude of the Burgers vector, $\rho_G = \sum_{\xi} \rho_G^{(\xi)}$ is the total GNDs density, and $\mathbf{t}^{(\xi)} \cdot \mathbf{t}^{(\xi)} = 1$.

Non-vanishing $\boldsymbol{\alpha}$ implies the existence of GNDs in the sense that the excess of dislocations of one sign, i.e. the net Burgers vector $\mathbf{b}$, in any region S bounded by a closed curve C, is given by Fleck et al. (1994), Fleck and Hutchinson (1997), Arsenlis and Parks (1999), and Bassani (2001)

$$b_i = \oint_C u_{i,p}^{\mathrm{p}} \, \mathrm{d}x_p = \int_S e_{jkl} u_{i,lk}^{\mathrm{p}} n_j \, \mathrm{d}A \tag{11}$$

where the Stokes' theorem is used to obtain the right part, $\mathbf{n}$ is the unit normal to surface S whose boundary is the curve C, and $\mathbf{e}$ is the permutation tensor. Thus, one obtains the Nye's dislocation density tensor $\boldsymbol{\alpha}$ as (Fleck and Hutchinson, 1997; Arsenlis and Parks, 1999; Bassani, 2001):

$$\alpha_{ij} = e_{jkl} u_{i,lk}^{\mathrm{p}} \tag{12}$$

such that $\boldsymbol{\alpha} = (\mathrm{curl}\boldsymbol{\varepsilon}^{\mathrm{p}})^{\mathrm{T}}$ where the superscript 'T' stands for the transpose. In the classical theory of isotropic plasticity the plastic spin

$$w_{ij}^{\mathrm{p}} = \frac{1}{2}(u_{i,j}^{\mathrm{p}} - u_{j,i}^{\mathrm{p}}) \tag{13}$$

is essentially irrelevant, as it may be absorbed by its elastic counterpart without affecting the resulting field equations (Gurtin and Anand, 2005). Therefore, by assuming irrotational plastic flow (i.e. $\mathbf{w}^{\mathrm{p}} = 0$ and $\nabla\mathbf{u}^{\mathrm{p}} = \boldsymbol{\varepsilon}^{\mathrm{p}}$), Eq. (12) can be written in terms of the plastic strain gradient $\nabla\boldsymbol{\varepsilon}^{\mathrm{p}}$ as

$$\alpha_{ij} = e_{jkl} \varepsilon_{il,k}^{\mathrm{p}} \tag{14}$$

By substituting Eq. (6) into Eq. (14), $\boldsymbol{\alpha}$ is written by Fleck et al. (1994), Fleck and Hutchinson (1997), Arsenlis and Parks (1999), Bassani (2001), and Bittencourt et al. (2003) as follows:

$$\alpha_{ij} = \sum_{\beta} p^{(\beta)}_{,k} \eta^{(\beta)}_{ikj} \tag{15}$$

where $\boldsymbol{\eta}$ is defined by

$$\eta^{(\beta)}_{ikj} = e_{jkl}\mu^{(\beta)}_{il} = \frac{1}{2} e_{jkl}(s^{(\beta)}_i n^{(\beta)}_l + n^{(\beta)}_i s^{(\beta)}_l) \tag{16}$$

Similarly, by taking the gradient of Eq. (6), one can write

$$\varepsilon^{\mathrm{p}}_{il,k} = \sum_{\beta} p^{(\beta)}_{,k} \mu^{(\beta)}_{il} \tag{17}$$

Therefore, Eq. (15) relates the dislocation density tensor to the slip gradients. Equating Eqs. (14) and (8) gives the gradient of plastic strain tensor in terms of GNDs density as

$$e_{jkl}\varepsilon^{\mathrm{p}}_{il,k} = \sum_{\xi} \rho^{(\xi)}_G b^{(\xi)}_i t^{(\xi)}_j \tag{18}$$

Similar to Eq. (9), one can also define the accumulation of GNDs, α, from Eq. (15) as follows:

$$\alpha = \sum_{\beta} \sum_{\xi} \sqrt{H^{(\beta,\zeta)} p^{(\beta)}_{,k} p^{(\xi)}_{,p} \eta^{(\beta)}_{ikj} \eta^{(\xi)}_{ipj}} \tag{19}$$

Neglecting the interaction among different slip systems gives

$$\alpha = \sum_{\beta} \sqrt{p^{(\beta)}_{,k} p^{(\beta)}_{,k}} \tag{20}$$

where $\boldsymbol{\eta}^{(\beta)}_{ikj} \boldsymbol{\eta}^{(\beta)}_{ipj} = \boldsymbol{\delta}_{kp}$. It can be seen that the accumulation of GNDs is related to the magnitude of plastic slip gradients. Equating Eqs. (10) and (20) gives the magnitude of plastic slip gradients in terms of the GNDs density as

$$\sum_{\beta} \sqrt{p^{(\beta)}_{,k} p^{(\beta)}_{,k}} = b\rho_G \tag{21}$$

Therefore, from Eqs. (18) and (21) one should consider the effects of both $\nabla\boldsymbol{\varepsilon}^{\mathrm{p}}$ and ∇p in the development of scale-dependent plasticity such that $\nabla\boldsymbol{\varepsilon}^{\mathrm{p}}$ and ∇p can not exist without the other and they introduce additional kinematic and isotropic hardenings, respectively. As shown above, the third-order tensor $(\nabla\boldsymbol{\varepsilon}^{\mathrm{p}})_{ijk} = \boldsymbol{\varepsilon}^{\mathrm{p}}_{ij,k}$ is attributed to a non-vanishing net Burgers vector at the microscale, while $(\nabla p)_k = p_{,k}$ is attributed to the accumulation of the GNDs. Both $\nabla\boldsymbol{\varepsilon}^{\mathrm{p}}$ and ∇p are considered in the following thermodynamic formulation as additional non-local state variables.

In classical continuum plasticity, the isotropic hardening variable (history variable), $\dot{p}$, is defined as the rate of the local effective plastic strain, which is intended to measure the SSD density and is expressed by

$$\dot{p} = \|\dot{\boldsymbol{\varepsilon}}^{\mathrm{p}}_{ij}\| = \sqrt{\dot{\boldsymbol{\varepsilon}}^{\mathrm{p}}_{ij}\dot{\boldsymbol{\varepsilon}}^{\mathrm{p}}_{ij}} \tag{22}$$

Substituting Eq. (6) into the above expression and neglecting interactions between different slip planes, yields $\dot{p} = \sum_{\beta}\dot{p}^{(\beta)}$. Therefore, in the following variational framework the local kinematic fields $\boldsymbol{\varepsilon}^{\mathrm{p}}_{ij}$ and p as well as the non-local kinematic fields $\boldsymbol{\varepsilon}^{\mathrm{p}}_{ij,k}$ and $p_{,k}$ are considered.

3. Thermodynamics of higher-order gradient plasticity

In order to be able to model the small-scale phenomena, such as the effect of size on the material mechanical properties and the width of the localization zones in softening media, an attempt is made now to account for the effect of non-uniform distribution of micro-defects on the homogenized response of the material. The main

issue is that the classical plasticity theory does not posses an intrinsic material length scale which makes it incapable of predicting such phenomena. Based on the discussion in the previous section, the dependence of the internal power on $\nabla\boldsymbol{\varepsilon}^{\mathrm{p}}$ and ∇p is the essential ingredient for the proposed strain gradient plasticity. Moreover, dependence on classical kinematic measures: the elastic strain tensor, $\boldsymbol{\varepsilon}^{\mathrm{e}}$, the plastic strain tensor, $\boldsymbol{\varepsilon}^{\mathrm{p}}$, and accumulation of plastic strain, p, is assumed.

In the classical continuum plasticity theory, one can define the unit direction of the plastic strain tensor as

$$N_{ij} = \frac{\dot{\varepsilon}^{\mathrm{p}}_{ij}}{\left\|\dot{\varepsilon}^{\mathrm{p}}_{ij}\right\|} = \frac{\dot{\varepsilon}^{\mathrm{p}}_{ij}}{\dot{p}} \Rightarrow \dot{\varepsilon}^{\mathrm{p}}_{ij} = \dot{p}N_{ij} \tag{23}$$

such that one writes

$$\|N_{ij}\| = N_{ij}N_{ij} = 1 \Rightarrow N_{ij}\frac{\dot{\varepsilon}^{\mathrm{p}}_{ij}}{\dot{p}} = 1 \Rightarrow \dot{p} = N_{ij}\dot{\varepsilon}^{\mathrm{p}}_{ip} \tag{24}$$

where Eq. $(23)_2$ corresponds to the normality flow rule to the yield surface f in the classical continuum plasticity theory, $\dot{\boldsymbol{\varepsilon}}^{\mathrm{p}} = \dot{\lambda}\partial f/\partial\boldsymbol{\sigma}$ where $\mathbf{N} = \partial f/\partial\boldsymbol{\sigma}$ and $\dot{p} = \dot{\lambda}$, similar to Eq. (6) in crystal plasticity theory. This is emphasized in Section 3.7.

One can write the following useful relation by taking the gradient of $\dot{p} = \sqrt{\dot{\boldsymbol{\varepsilon}}^{\mathrm{p}}_{ij}\dot{\boldsymbol{\varepsilon}}^{\mathrm{p}}_{ij}}$ such that

$$\dot{p}_{,k} = \frac{\dot{\varepsilon}^{\mathrm{p}}_{ij}\dot{\varepsilon}^{\mathrm{p}}_{ij,k}}{\sqrt{\dot{\varepsilon}^{\mathrm{p}}_{mn}\dot{\varepsilon}^{\mathrm{p}}_{mn}}} = \frac{\dot{\varepsilon}^{\mathrm{p}}_{ij}}{\dot{p}}\dot{\varepsilon}^{\mathrm{p}}_{ij,k} = N_{ij}\dot{\varepsilon}^{\mathrm{p}}_{ij,k} \tag{25}$$

where Eq. $(23)_1$ is utilized. Moreover, one can notice from Eqs. $(24)_3$ and (25) that

$$N_{ij,k}\dot{\varepsilon}^{\mathrm{p}}_{ij} = 0_k \tag{26}$$

where $\mathbf{0}$ is a zero vector. The result in Eq. (26) implies that $\nabla\mathbf{N}$ is normal to $\dot{\boldsymbol{\varepsilon}}^{\mathrm{p}}$.

Equivalently, one can also obtain the above result by operating on the identity $N_{ij}N_{ij} = 1$, Eq. $(24)_1$, by the gradient, which yields

$$N_{ij,k}N_{ij} + N_{ij}N_{ij,k} = 0_k \Rightarrow N_{ij,k}N_{ij} = 0_k \tag{27}$$

Multiplying both sides of Eq. $(27)_2$ by $\dot{p}$ and using the result in Eq. $(23)_2$ yields Eq. (26).

It is noteworthy that at the crystal level one can express $\nabla\boldsymbol{\varepsilon}^{\mathrm{p}}$ by Eq. (17) directly from Eq. (6) such that $\nabla\boldsymbol{\mu}^{(\beta)} = 0$. However, for polycrystals, operating in Eq. $(23)_2$ by the gradient yields

$$\dot{\varepsilon}^{\mathrm{p}}_{ij,k} = \dot{p}_{,k}N_{ij} + \dot{p}N_{ij,k} \tag{28}$$

such that $\nabla\mathbf{N} \neq 0$.

In continuum plasticity, the generalized rate of total accumulation of the plastic strain and plastic strain gradients can thus be defined as (e.g. Fleck and Hutchinson, 2001; Gurtin, 2003; Gudmundson, 2004):

$$\dot{E}^{\mathrm{p}2} = \dot{p}^2 + \ell^2\dot{p}_{,k}\dot{p}_{,k} = \dot{\varepsilon}^{\mathrm{p}}_{ij}\dot{\varepsilon}^{\mathrm{p}}_{ij} + A_{ijmn}\dot{\varepsilon}^{\mathrm{p}}_{ij,k}\dot{\varepsilon}^{\mathrm{p}}_{mn,k} \tag{29}$$

where Eq. (25) is used in obtaining the second part, $A_{ijmn} = \ell^2 N_{ij}N_{mn}$ with ℓ is the material length scale parameter used for dimensional consistency, and E^{p} is the non-local effective plastic strain, which is intended to measure the total dislocation density combining both SSDs and GNDs. With the absence of plastic strain gradients, E^{p} reduces to the local effective plastic strain p. Hence, the authors believe that for a proper constitutive description at small length scales, the internal power and the Helmholtz free energy should not include only the effects of $\boldsymbol{\varepsilon}^{\mathrm{p}}$ and p but should also include the effects of $\nabla\boldsymbol{\varepsilon}^{\mathrm{p}}$ and ∇p. Although these variables have a common origin in dislocation storage and motion, they will be treated independent of each other. This gives different physical interpretations that guide one to different evolution equations and allowing one to computationally introduce the influence of one scale on the other (e.g. the effect of mesoscale on macroscale). For example dislocation interactions are observed on a mesolevel with a length scale 0.1–10 μm affecting strongly the material behavior on the macrolevel with a length scale $\geqslant$100 μm. However, those variables are considered here mathematically related to their local counterparts and, therefore, special care must be taken to properly account for their coupling.

Some authors have considered in their variational formation only the gradient of the plastic strain tensor, $\nabla\boldsymbol{\varepsilon}^{\mathrm{p}}$, and others have considered only the gradient of the effective plastic strain, ∇p. But, to the authors' best knowledge, no one has really considered the effect of both $\nabla\boldsymbol{\varepsilon}^{\mathrm{p}}$ and ∇p in the variational formulation. For example, Shizawa and Zbib (1999), Mentzel and Steinmann (2000), Gao et al. (1999), Fleck and Hutchinson (2001), Gurtin (2003, 2004), Gurtin and Anand (2005), and Gudmundson (2004) have developed gradient theories that allow dependences on $\nabla\boldsymbol{\varepsilon}^{\mathrm{p}}$ only. However, the theories of Fleck and Hutchinson (2001) and Gao et al. (1999) introduce gradients in the plastic strain that only affect the isotropic hardening part with no kinematic hardening. The pioneering continuum gradient plasticity theories of Gurtin (2003, 2004) and Gurtin and Anand (2005), do not incorporate ∇p in the principle of virtual power, but is incorporated in the functional dependence of the Helmholtz free energy and as a constitutive assumption. Mühlhaus and Aifantis (1991), Polizzotto and Borino (1998), Acharya and Bassani (2000), Liebe and Steinmann (2001), Voyiadjis and Abu Al-Rub (2004), and Abu Al-Rub and Voyiadjis (2006, in press) have developed gradient theories that allow dependences on ∇p such that only the isotropic hardening part is affected by the presence of these gradients. Voyiadjis et al. (2001, 2003, 2004) have introduced first and second order gradients in both isotropic and kinematic hardenings. However, the kinematic hardening is introduced through an arbitrary flux variable and not the plastic strain. In this work both $\nabla\boldsymbol{\varepsilon}^{\mathrm{p}}$ and ∇p enter the definitions of the internal virtual power and the Helmholtz free energy. Therefore, one can anticipate that the conjugate force of $\nabla\boldsymbol{\varepsilon}^{\mathrm{p}}$ is the non-local backstress while the conjugate force of ∇p is the non-local drag stress. This will be shown in the following sections of this paper.

The formulation of a continuum-based plasticity model requires the satisfaction of the axioms of equilibrium and thermodynamics. The following sections present the principle of virtual power and the fundamental statements of irreversible thermodynamics that are commonly used in the mathematical modeling of the material mechanical behavior.

3.1. Principle of virtual power: macroscopic and microscopic force balances

The principle of virtual power is the assertion that, given any sub-body Γ, the virtual power expended on Γ by materials or bodies exterior to Γ (i.e. external power) be equal to the virtual power expended within Γ (i.e. internal power). Let $\mathbf{n}$ denotes the outward unit normal to $\partial\Gamma$. The external expenditure of power is assumed to arise from a macroscopic body force $\mathbf{b}$, a macroscopic surface traction $\mathbf{t}$, the microtraction stress tensor conjugate to $\dot{\boldsymbol{\varepsilon}}^{\mathrm{p}}$, and the microtraction force associated with the history plasticity variable $\dot{p}$. One, therefore, can write the external virtual power in the following form:

$$P_{\mathrm{ext}} = \int_{\Gamma} b_i \delta v_i \,\mathrm{d}V + \int_{\partial\Gamma} t_i \delta v_i \,\mathrm{d}A - \int_{\Gamma} \rho \dot{v}_i \delta v_i \,\mathrm{d}V + \int_{\partial\Gamma} m_{ij} \delta \dot{\varepsilon}^{\mathrm{p}}_{ij} \,\mathrm{d}A + \int_{\partial\Gamma} q \delta \dot{p} \,\mathrm{d}A \tag{30}$$

The kinematical fields $\delta\boldsymbol{v}$, $\delta\dot{\boldsymbol{\varepsilon}}^{\mathrm{p}}$, and $\delta\dot{p}$ are considered here as virtual, where δ is the variation parameter, ρ is the mass density, $\boldsymbol{v}$ is the velocity vector, and $\dot{\mathbf{v}}$ is the acceleration vector. The tensor $\mathbf{m}$ is the microtraction stress tensor conjugate to $\boldsymbol{\varepsilon}^{\mathrm{p}}$, defined for each unit vector $\mathbf{n}$ normal on the boundary $\partial\Gamma$ of Γ. The scalar q is the microtraction force associated with the effective plastic strain variable, p. The micro-stresses q and $\mathbf{m}$ are precisely those introduced, respectively, by Fleck and Hutchinson (2001) as a conjugate to ∇p and Gurtin [e.g. Gurtin (2003, 2004) and Gurtin and Anand (2005)] as a conjugate to $\nabla\boldsymbol{\varepsilon}^{\mathrm{p}}$ in their representation of a variational principle governing the one-non-local-parameter theory. Therefore, the first three integrals in Eq. (30) constitute the macroscopic power expenditure, while the last two terms constitute the microscopic power expenditure. Moreover, since plastic deformation, accommodated by dislocation generation and motion, is affected by interfaces, the last two integrals result in higher-order boundary conditions generally consistent with the framework of a gradient-type theory. These extra boundary conditions need to be imposed at external and internal boundary surfaces or interfaces separating different constituents as is shown later in Section 3.4.

The external power is balanced by an internal expenditure of power characterized by an elastic stress $\boldsymbol{\sigma}$ defined over Γ for all time, the backstress $\mathbf{X}$ associated with kinematic hardening, and the drag-stress R associated with isotropic hardening. However, since the goal of this paper is a theory that allows for gradients of the plastic strain and effective plastic strain, one also considers power expenditures associated with kinematic variables $\nabla\boldsymbol{\varepsilon}^{\mathrm{p}}$ and ∇p. One, therefore, assume that additional power is expended internally by the higher-order

microstress $\mathbf{S}$ conjugate to $\nabla\boldsymbol{\varepsilon}^{\mathrm{p}}$, and the higher-order microforce vector $\mathbf{Q}$ conjugate to ∇p. Specifically, the internal virtual power is assumed to have the following form:

$$P_{\mathrm{int}} = \int_{\Gamma} \left(\sigma_{ij}\delta\dot{\varepsilon}^{\mathrm{e}}_{ij} + X_{ij}\delta\dot{\varepsilon}^{\mathrm{p}}_{ij} + R\delta\dot{p} + S_{ijk}\delta\dot{\varepsilon}^{\mathrm{p}}_{ij,k} + Q_k\delta\dot{p}_{,k} \right) \mathrm{d}V \tag{31}$$

and to balance P_{ext}, Eq. (30), in the sense that

$$P_{\mathrm{ext}} = P_{\mathrm{int}} \tag{32}$$

The first three terms in Eq. (31) constitutes the definition of the local internal virtual power in the mathematical definition of standard plasticity theory. The second term represents the internal power generated by the backstress $\mathbf{X}$ (or the residual-stress) attributed to kinematic hardening in order to introduce anisotropic effects. A kinematic variable which is often used is the plastic strain itself, $\boldsymbol{\varepsilon}^{\mathrm{p}}$, as for example, in Prager's hardening model (linear kinematic hardening). However, a more general flux tensor associated with backstress may be assumed (Voyiadjis et al., 2001, 2003, 2004). The third term in Eq. (31) represents the internal power generated by the drag-stress R which causes isotropic hardening. The last two terms in Eq. (31) are meant to take into account the large spatial variations in $\boldsymbol{\varepsilon}^{\mathrm{p}}$ at small length scales. The first term represents the internal power generated by the non-local backstress $\mathbf{S}$ such that it introduces additional kinematic hardening through a non-vanishing net Burgers vector. The third-order tensor $\mathbf{S}$ also follows precisely that introduced by Gurtin (2000, 2002, 2003, 2004) in his thermodynamics of one-parameter theory $\nabla\boldsymbol{\varepsilon}^{\mathrm{p}}$. The last term in Eq. (31) represents the internal power generated by the non-local drag vector $\mathbf{Q}$ which is meant to account for the additional isotropic hardening from the accumulation of GNDs. This may give satisfactory consideration of the large variations in plasticity defects at the micro-scale.

Eq. (31) is based on the concepts that the power expended by each kinematical field be expressible in terms of an associated force system consistent with its own balance. However, these kinematical fields are no longer independent and, therefore, special care is taken in the following in order to properly account for their coupling. Moreover, it is noteworthy that one might argue that the above energetic balance might best be characterized through a dependence of P_{int} on the (scalar) accumulation of the plastic strain p (internal history variable) and not on the plastic strain itself $\boldsymbol{\varepsilon}^{\mathrm{p}}$. But the effects of the two variables are different: a dependence of P_{int} on $\boldsymbol{\varepsilon}^{\mathrm{p}}$ gives rise to kinematic hardening; while a dependence of P_{int} on p gives rise to isotropic hardening. Similar argument applies to $\nabla\boldsymbol{\varepsilon}^{\mathrm{p}}$ and ∇p.

Now substituting the relation $\dot{\boldsymbol{\varepsilon}}^{\mathrm{e}} = \dot{\boldsymbol{\varepsilon}} - \dot{\boldsymbol{\varepsilon}}^{\mathrm{p}}$, and Eqs. $(24)_3$ and (25) into Eq. (31) along with

$$\delta\dot{p} = \delta(\dot{\varepsilon}^{\mathrm{p}}_{ij}N_{ij}) = N_{ij}\delta\dot{\varepsilon}^{\mathrm{p}}_{ij} + \dot{\varepsilon}^{\mathrm{p}}_{ij}\delta N_{ij} \quad \text{and} \quad \delta\dot{p}_{,k} = \delta(\dot{\varepsilon}^{\mathrm{p}}_{ij,k}N_{ij}) = N_{ij}\delta\dot{\varepsilon}^{\mathrm{p}}_{ij,k} + \dot{\varepsilon}^{\mathrm{p}}_{ij,k}\delta N_{ij} \tag{33}$$

yields

$$P = \int_{\Gamma} [\sigma_{ij}\delta\dot{\varepsilon}_{ij} - (\tau_{ij} - X_{ij} - RN_{ij})\delta\dot{\varepsilon}^{\mathrm{p}}_{ij} + (S_{ijk} + Q_kN_{ij})\delta\dot{\varepsilon}^{\mathrm{p}}_{ij,k} + (R\dot{\varepsilon}^{\mathrm{p}}_{ij} + Q_k\dot{\varepsilon}^{\mathrm{p}}_{ij,k})\delta N_{ij}]\,\mathrm{d}V \tag{34}$$

where due to plastic incompressibility, one can easily prove that $\boldsymbol{\sigma} : \dot{\boldsymbol{\varepsilon}} = \boldsymbol{\tau} : \dot{\boldsymbol{\varepsilon}}$ where $\tau_{ij} = \sigma_{ij} - \frac{1}{3}\sigma_{kk}\delta_{ij}$ is the deviatoric component of the Cauchy stress tensor $\boldsymbol{\sigma}$. By applying the divergence theorem, one can rewrite Eq. (34) as follows:

$$\begin{aligned} P_{\mathrm{int}} = &- \int_{\Gamma} \sigma_{ij,j}\delta v_i\,\mathrm{d}V - \int_{\Gamma} \left[\tau_i j - X_{ij} + S_{ijk,k} + Q_kN_{ij,k} - (R - Q_{k,k})N_i j\right]\delta\dot{\varepsilon}^{\mathrm{p}}_{ij}\,\mathrm{d}V \\ &+ \int_{\Gamma} (R\dot{\varepsilon}^{\mathrm{p}}_{ij} + Q_k\dot{\varepsilon}^{\mathrm{p}}_{ij,k})\delta N_{ij}\,\mathrm{d}V + \int_{\partial\Gamma} \sigma_{ij}n_j\delta v_i\,\mathrm{d}A + \int_{\partial\Gamma} \left[S_{ijk} + Q_kN_{ij}\right]n_k\delta\dot{\varepsilon}^{\mathrm{p}}_{ij}\,\mathrm{d}A \end{aligned} \tag{35}$$

Moreover, Eq. (30) can be rewritten by substituting Eq. $(24)_3$ as

$$P_{\mathrm{ext}} = \int_{\Gamma} (b_i - \rho\dot{v}_i)\delta v_i\,\mathrm{d}V + \int_{\partial\Gamma} t_i\delta v_i\,\mathrm{d}A + \int_{\partial\Gamma} (m_{ij} + qN_{ij})\delta\dot{\varepsilon}^{\mathrm{p}}_{ij}\,\mathrm{d}A + \int_{\partial\Gamma} q\dot{\varepsilon}^{\mathrm{p}}_{ij}\delta N_{ij}\,\mathrm{d}A \tag{36}$$

By applying the axiom of equilibrium of the principle of virtual power to the region Γ, Eq. (32), one obtains the following equilibrium equation:

$$\int_{\Gamma}(\sigma_{ij,j}+b_i-\rho\dot{v}_i)\delta v_i\,\mathrm{d}V+\int_{\partial\Gamma}(t_i-\sigma_{ij}n_j)\delta v_i\,\mathrm{d}A+\int_{\partial\Gamma}\left[(m_{ij}+qN_{ij})-(S_{ijk}+Q_kN_{ij})n_k\right]\delta\dot{\varepsilon}^{\mathrm{p}}_{ij}\,\mathrm{d}A$$
$$+\int_{\Gamma}\left[\tau_{ij}-X_{ij}+S_{ijk,k}+Q_kN_{ij,k}-(R-Q_{k,k})N_{ij}\right]\delta\dot{\varepsilon}^{\mathrm{p}}_{ij}\,\mathrm{d}V-\int_{\Gamma}(R\dot{\varepsilon}^{\mathrm{p}}_{ij}+Q_k\dot{\varepsilon}^{\mathrm{p}}_{ij,k})\delta N_{ij}\,\mathrm{d}V$$
$$+\int_{\partial\Gamma}q\dot{\varepsilon}^{\mathrm{p}}_{ij}\delta N_{ij}\,\mathrm{d}A=0 \tag{37}$$

However, similar to the result in Eq. (26), one can easily show by operating on the identity $N_{ij}N_{ij}=1$, Eq. $(24)_1$, by δ along with Eq. $(23)_1$ the following:

$$\dot{\varepsilon}^{\mathrm{p}}_{ij}\delta N_{ij}=0 \tag{38}$$

By taking the gradient of the above equation, one can write

$$\dot{\varepsilon}^{\mathrm{p}}_{ij}\delta N_{ij,k}=-\dot{\varepsilon}^{\mathrm{p}}_{ij,k}\delta N_{ij} \tag{39}$$

Moreover, operating on Eq. (26) by δ gives

$$\dot{\varepsilon}^{\mathrm{p}}_{ij}\delta N_{ij,k}=-N_{ij,k}\delta\dot{\varepsilon}^{\mathrm{p}}_{ij} \tag{40}$$

Comparing Eqs. (39) and (40) yields the following useful result:

$$\dot{\varepsilon}^{\mathrm{p}}_{ij,k}\delta N_{ij}=N_{ij,k}\delta\dot{\varepsilon}^{\mathrm{p}}_{ij} \tag{41}$$

Now substituting the results in Eqs. (38) and (41) into the virtual power balance, Eq. (37), yields the following expression:

$$\int_{\Gamma}(\sigma_{ij,j}+b_i-\rho\dot{v}_i)\delta v_i\,\mathrm{d}V+\int_{\sigma\Gamma}(t_i-\sigma_{ij}n_j)\delta v_i\,\mathrm{d}A+\int_{\Gamma}[\tau_{ij}-X_{ij}+S_{ijk,k}-(R-Q_{k,k})N_{ij}]\delta\dot{\varepsilon}^{\mathrm{p}}_{ij}\,\mathrm{d}V$$
$$+\int_{\partial\Gamma}\left[(m_{ij}+qN_{ij})-(S_{ijk}+Q_kN_{ij})n_k\right]\delta\dot{\varepsilon}^{\mathrm{p}}_{ij}\,\mathrm{d}A=0 \tag{42}$$

The fields Γ, $\delta\mathbf{v}$, and $\delta\dot{\boldsymbol{\varepsilon}}$ may be arbitrarily specified if and only if

$$\sigma_{ij,j}+b_i=\rho\dot{v}_i \text{ (macroforce balance)} \tag{43}$$
$$t_i=\sigma_{ij}n_j \text{ (macrotraction condition)} \tag{44}$$
$$\tau_{ij}-X_{ij}+S_{ijk,k}-(R-Q_{k,k})N_{ij}=0 \text{ (non-local microforce balance)} \tag{45}$$
$$\tilde{m}_{ij}=(S_{ijk}+Q_kN_{ij})n_k \text{(microtraction condition)} \tag{46}$$

such that $\tilde{\mathbf{m}}=\mathbf{m}+q\mathbf{N}$. Eq. (43) expresses the local static or dynamic equilibrium or the macroforce balance according to the notion of Gurtin (2003). Eq. (44) defines the stress vector as the surface density of the forces introduced. It shows that $\boldsymbol{\sigma}$ is really the Cauchy stress tensor, which is a second-order symmetric tensor. It also provides the local macrotraction 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. However, one can view the microforce balance in Eq. (45) as the plasticity non-local yield condition, which is demonstrated in the next section, and the microtraction condition in Eq. (46) as a higher-order condition (or internal boundary condition) augmented by the interaction of dislocations across interfaces (Gurtin, 2003; Gudmundson, 2004).

It is noteworthy to mention that since $\tilde{\mathbf{m}}=\mathbf{m}+q\mathbf{N}$, one may assume that the microtraction conditions, Eq. (46), can be rewritten using two separate conditions such that

$$m_{ij}=S_{ijk}n_k,\quad q=Q_kn_k \tag{47}$$

where the former imposes constraints on the flow of dislocations through interfaces, while the later imposes constraints on the dislocation pileups at interfaces. However, both $\dot{\boldsymbol{\varepsilon}}^{\mathrm{p}}$ and $\dot{p}$ are depended and related to each other through Eq. $(24)_3$. Therefore, at this stage it appears that Eq. (46) is more appropriate. This topic will be thoroughly investigated in a future work.

3.2. Non-local yield criterion

In the following it will be shown that the microforce balance presented in Eq. (45) is nothing more than the non-local yield condition.

By taking the Euclidean norm $\|\|$ of Eq. (45), one can write

$$\|\tau_{ij} - X_{ij} + S_{ijk,k}\| - \|R - Q_{k,k}\|\|N_{ij}\| = 0 \tag{48}$$

where $\mathbf{N}$ is collinear with $\boldsymbol{\tau} - \mathbf{X} + \operatorname{div}\mathbf{S}$. Moreover, since $\|R - Q_{k,k}\| = R - Q_{k,k}$ and $\|N_{ij}\| = 1$, one can then rewrite the above expression as the non-local yield criterion or the non-local plasticity loading surface f such that

$$f = \left\|\tau_{ij} - X_{ij} + S_{ijk,k}\right\| - R + Q_{k,k} = 0 \tag{49}$$

It is obvious that Eq. (49) represents a sphere in deviatoric stress-space of radius $R - \operatorname{div}\mathbf{Q}$ centered at $\mathbf{X} - \operatorname{div}\mathbf{S}$. One can also notice that the higher-order stress $\operatorname{div}\mathbf{S}$ is a back-stress quantity giving rise to additional kinematic hardening, while the microstress $\operatorname{div}\mathbf{Q}$ is giving rise to additional isotropic hardening.

Since Eq. (49) implies that $\mathbf{N}$ is parallel to $\boldsymbol{\tau} - \mathbf{X} + \operatorname{div}\mathbf{S}$, one can, therefore, express the direction of plastic strain, $\mathbf{N}$, as follows:

$$N_{ij} = \frac{\tau_{ij} - X_{ij} + S_{ijk,k}}{\|\tau_{mn} - X_{mn} + S_{mnp,p}\|} \tag{50}$$

Or equivalently, one can rewrite Eq. (50) from Eq. (49) as follows:

$$N_{ij} = \frac{\tau_{ij} - X_{ij} + S_{ijk,k}}{R - Q_{k,k}} \tag{51}$$

Substituting Eq. $(23)_2$ into the above expression, one can easily write the following expression for the plasticity flow rule:

$$\dot{\varepsilon}^{\mathrm{p}}_{ij} = \dot{p}\frac{\tau_{ij} - X_{ij} + S_{ijk,k}}{R - Q_{k,k}} \tag{52}$$

or equivalently, the flow rule in Eq. (52) can be expressed from Eq. (50) as follows:

$$\dot{\varepsilon}^{\mathrm{p}}_{ij} = \dot{p}\frac{\tau_{ij} - X_{ij} + S_{ijk,k}}{\|\tau_{mn} - X_{mn} + S_{mnp,p}\|} \tag{53}$$

Therefore, one can easily proof that the plasticity flow rule can be written as

$$\dot{\varepsilon}^{\mathrm{p}}_{ij} = \dot{p}\frac{\partial f}{\partial \sigma_{ij}} = -\dot{p}\frac{\partial f}{\partial X_{ij}} = \dot{p}\frac{\partial f}{\partial S_{ijk,k}} \tag{54}$$

such that

$$N_{ij} = \frac{\partial f}{\partial \sigma_{ij}} = -\frac{\partial f}{\partial X_{ij}} = \frac{\partial f}{\partial S_{ijk,k}} \tag{55}$$

Therefore, the flow rule in Eq. (54) asserts that the flow direction $\mathbf{N}$ in Eq. (55) is normal to the yield surface and directed outward from the yield surface. Moreover, if the higher-order gradients are neglected, one can easily retrieve from Eqs. (49), (54) and (55), respectively, the classical yield criterion, flow rule, and flow direction.

A direct consequence of the above formalism is that the non-local yield function, Eq. (49) can be derived from the principle of virtual power.

3.3. Non-local Clausius–Duhem inequality

Utilizing the derived microforce balance, Eq. (45), and the microtraction condition, Eq. (46), into Eq. (35), and replacing the virtual quantities by the actual fields, one can rewrite the expression of the internal power defined in Eq. (31) as follows:

$$P_{\text{int}} = \int_{\Gamma} \sigma_{ij}\dot{\varepsilon}_{ij}\,\mathrm{d}V + \int_{\partial\Gamma} \tilde{m}_{ij}\dot{\varepsilon}^{\text{p}}_{ij}\,\mathrm{d}A \tag{56}$$

Comparing the above equation with its corresponding local expression in Green and Naghdi (1971), implies that the long-range (non-local) energy interactions can be of non-vanishing within the plastic zone, which is represented by the second term in Eq. (56). Hence, according to the notion of Eringen and Edelen (1972), the energy term $\int_{\partial\Gamma} \tilde{\mathbf{m}}_{ij}\dot{\boldsymbol{\varepsilon}}^{\text{p}}_{ij}\,\mathrm{d}A$ is called as the *non-locality energy residual* that results from microstructural interactions between the material points in the active plastic zone and at interfaces. Therefore, one can define the density of the non-locality energy residual, $\mathbb{R}$, as follows:

$$\int_{\Gamma} \mathbb{R}\,\mathrm{d}V = \int_{\partial\Gamma} \tilde{m}_{ij}\dot{\varepsilon}^{\text{p}}_{ij}\,\mathrm{d}A = \int_{\partial\Gamma} (S_{ijk} + Q_k N_{ij}) n_k \dot{\varepsilon}^{\text{p}}_{ij}\,\mathrm{d}A \tag{57}$$

By applying the divergence theorem to Eq. (57) along with Eq. (46), one obtains

$$\int_{\Gamma} \mathbb{R}\,\mathrm{d}V = \int_{\Gamma} [\mathbb{Z}_{ijk}\dot{\varepsilon}^{\text{p}}_{ij}]_{,k}\,\mathrm{d}V \tag{58}$$

where

$$\mathbb{Z}_{ijk} = S_{ijk} + Q_k N_{ij} \tag{59}$$

such that $\mathbb{R}$ is given by

$$\mathbb{R} = [\mathbb{Z}_{ijk}\dot{\varepsilon}^{\text{p}}_{ij}]_{,k} = \mathbb{Z}_{ijk,k}\dot{\varepsilon}^{\text{p}}_{ij} + \mathbb{Z}_{ijk}\dot{\varepsilon}^{\text{p}}_{ij,k} \tag{60}$$

where $\mathbb{R} \neq 0$ in Γ^{p}, but $\mathbb{R} = 0$ out of Γ^{p} or for a homogeneous plastic deformation (i.e. $\mathbb{R} = 0$ in the absence of plastic strain gradients).

One considers here 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 power done by external forces (Gurtin, 2000). If one denotes $\rho\Psi$ as the specific free energy, this requirement takes the form of a free energy inequality

$$\overset{\bullet}{\int_{\Gamma} \rho\Psi\,\mathrm{d}V} \leqslant P_{\text{ext}} \tag{61}$$

From the conservation of mass law, one can write $\overset{\bullet}{\int_{\Gamma} \rho\Psi\,\mathrm{d}V} = \int_{\Gamma} \rho\dot{\Psi}\,\mathrm{d}V$. By substituting Eqs. (56) and (57) into Eq. (61), one obtains the following thermodynamic restriction in a point wise form:

$$\sigma_{ij}\dot{\varepsilon}_{ij} - \rho\dot{\Psi} + \mathbb{R} \geqslant 0 \tag{62}$$

The inequality in Eq. (62) is termed here as the *non-local Clausius–Duhem inequality* differing from its classical counterpart only in the presence of $\mathbb{R}$. This inequality holds everywhere in Γ, but $\mathbb{R} = 0$ at material points in the elastic zone. Moreover, it can be noted from Eq. (60) that for a homogeneous plastic strain distribution $\mathbb{R} = 0$, one retains the classical Clausius–Duhem inequality.

The non-local Clausius–Duhem inequality, Eq. (62), can be recognized to be substantially coincident with the analogous inequality presented by Polizzotto and Borino (1998). This result credits the proposed framework as a valid approach to model non-local plasticity. Therefore, for more details on the nature of the non-locality residual $\mathbb{R}$ the reader is referred to the work by Polizzotto and Borino (1998). However, the framework used here to evaluate the non-locality residual $\mathbb{R}$ is more thermodynamically based than that used by Polizzotto and Borino (1998).

In Section 3.5 the non-local Clausius–Duhem inequality in Eq. (62) will be employed for deriving the thermodynamic restrictions upon the inherent constitutive equations, to be satisfied for any admissible deformation mechanism.

3.4. Microlevel plastic boundary conditions

Polizzotto (e.g. Polizzotto and Borino, 1998; Polizzotto, 2003) assumed that the non-locality residual in Eq. (57) is equal to zero and called it as the *insulation condition* meaning that non-local energy is not allowed to

flow from any point in Γ to the exterior of the body. Therefore, if one neglects the interior surface energy that results from dislocation interactions at the surface/interface boundaries (e.g. internal boundaries at inclusions), the *insulation condition* of Polizzotto can be expressed as

$$\int_{\Gamma} \mathbb{R}\, \mathrm{d}V = 0 \tag{63}$$

Furthermore, one retrieves the classical definition of the internal power if the non-locality energy residual is simply set zero in Eq. (56). Therefore, from the above tow arguments, one may require the application of internal micro-boundary conditions in a pointwise format *if there is no plastic flow across the interfaces*, which results in a null expenditure of micro-power in the sense that:

$$\tilde{m}_{ij}\dot{\varepsilon}^{\mathrm{p}}_{ij} = 0 \quad \text{on } \partial\Gamma^{\mathrm{p}} \tag{64}$$

where $\partial\Gamma^{\mathrm{p}} \subseteq \partial\Gamma$ is the plastic boundary. The above equation renders two conditions according to a split of the plastic subdomain boundary into external and internal parts, $\partial\Gamma^{\mathrm{p}} = \partial\Gamma^{\mathrm{p}}_{\mathrm{int}} \cup \partial\Gamma^{\mathrm{p}}_{\mathrm{ext}}$:

(a) *Microplastic-clamped* boundary condition that is imposed on the internal plastic boundary $\partial\Gamma^{\mathrm{p}}_{\mathrm{int}}$ such that

$$\dot{\varepsilon}^{\mathrm{p}}_{ij} = \mathbf{0} \quad \text{on } \partial\Gamma^{\mathrm{p}}{}_{\mathrm{int}} \tag{65}$$

and gives the so-called continuity boundary condition of Dirichlet type and is meant to characterize, for example, microscopic behavior at the boundary of a metallic film perfectly bonded to an elastic substrate or metallic matrix perfectly bonded to an elastic inclusion. This condition arises from the consideration that in general the stress rate $\dot{\boldsymbol{\sigma}}$ is continuous across $\partial\Gamma^{\mathrm{p}}_{\mathrm{int}}$ and thus the related elastic strain rate, $\dot{\boldsymbol{\varepsilon}}^{\mathrm{e}}$, and plastic strain rate, $\dot{\boldsymbol{\varepsilon}}^{\mathrm{p}}$, must be continuous. Therefore, this boundary condition places a constraint on the plastic flow and could characterize the dislocation blocking at the interface. Moreover, $\partial\Gamma^{\mathrm{p}}_{\mathrm{int}}$ could characterize the movable elastic-plastic boundary.

(b) *Microtraction-free* boundary condition that is imposed on the external plastic boundary $\partial\Gamma^{\mathrm{p}}_{\mathrm{ext}} \subseteq \partial\Gamma$

$$\tilde{m}_{ij} = \mathbf{0} \quad \text{on } \partial\Gamma^{\mathrm{p}}_{\mathrm{ext}} \tag{66}$$

and gives the so-called Neumann type boundary which is the simplest form of Eq. (46) and assumes that the microtractions $\tilde{\mathbf{m}}$ vanish at the external surfaces $\partial\Gamma^{\mathrm{p}}_{\mathrm{ext}} = \partial\Gamma^{\mathrm{p}} \bigcap \partial\Gamma$ (i.e. unmovable external surfaces). This condition is meant to characterize, for example, the free surface of a void in a material or the free surfaces of nano-size structural systems. Eq. (66) places no constraint on the plastic flow and could characterize free dislocation movements across the boundaries. Moreover, in case of external surface tractions the macrotractions $\mathbf{t}$ in Eq. (44) has a value whereas the microtractions $\tilde{\mathbf{m}}$ could vanish.

The above null boundary conditions for microscopically hard and microscopically free portions of $\partial\Gamma^{\mathrm{p}}$ have also been introduced by Gurtin (e.g. Gurtin, 2000, 2002, 2003, 2004) and Fleck and Hutchinson (2001). However, these conditions are very difficult to be satisfied in reality, particularly, for large surface-to-volume ratios which the gradient plasticity theories are mainly intended to characterize. Therefore, these boundary conditions ignore the non-locality residual $\int_{\Gamma} \mathbb{R}\ \mathrm{d}V$ at free surfaces and interfaces. However, surface energy, which can be characterized by the non-locality energy residual as shown next, is significant and cannot be ignored when the surface-to-volume ratio becomes large enough. At the micron and higher length scales, the surface-to-volume ratio is small enough and can be neglected and indeed the above boundary conditions hold true. However, for submicron and smaller length scales the surface-to-volume ratio is appreciable. Here, $\tilde{\mathbf{m}}$ is meant to be the driving force at the material internal and external boundaries such that for an intermediate (i.e. not free and not clamped) kind of microscopic boundary condition, one has $\tilde{\mathbf{m}} \neq \mathbf{0}$ on $\partial\Gamma^{\mathrm{p}}_{\mathrm{ext}}$ and $\dot{\boldsymbol{\varepsilon}} \neq \mathbf{0}$ on $\partial\Gamma^{\mathrm{p}}{}_{\mathrm{int}}$. Therefore, microtraction stress $\tilde{\mathbf{m}}$ can be interpreted as the *surface stress* at free or interface surfaces which is conjugate to the surface plastic strain. The physical dimensions of the components of $\tilde{\mathbf{m}}$ are force/length. This aspect of the gradient theory could be the appropriate approach to extend its applicability beyond the submicron scale size effects to the nano scale size effects.

One now considers the case if the surface $\partial\Gamma^{\mathrm{p}}$ is an interface with an elastic or rigid surface, where dislocations pileup, $\tilde{\mathbf{m}}$ can be interpreted as the conjugate force to $\boldsymbol{\varepsilon}^{\mathrm{p}}$ at the interface (e.g. Gudmundson, 2004; Sharma and Ganti, 2004; Dingrevillea et al., 2005). If this situation rises, it can be modeled by a surface energy that depends on the plastic strain state at the interface of the plastically deforming material. This surface energy accounts for energy due to interfaces between distinct phase regions. The microtraction stress $\tilde{\mathbf{m}}$ can then be related to the surface energy as follows (e.g. Gudmundson, 2004; Sharma and Ganti, 2004; Dingrevillea et al., 2005):

$$\tilde{m}_{ij} = \frac{\partial\varphi(\varepsilon^{\mathrm{p}})}{\partial\varepsilon_{ij}^{\mathrm{p}(s)}} \quad \text{on } \partial\Gamma^{\mathrm{p}} \tag{67}$$

where φ is the surface energy per unit surface area, which is a plastic deformation-dependent, and $\boldsymbol{\varepsilon}^{\mathrm{p}(S)}$ is the surface plastic strain. Continuity of the strain field requires $\boldsymbol{\varepsilon}^{\mathrm{p}} = \boldsymbol{\varepsilon}^{\mathrm{p}(S)}|_{\partial\Gamma}$ at the interface. The components of $\boldsymbol{\varepsilon}^{\mathrm{p}(S)}$ are the extensional and shear plastic strains with respect to a locally rectangular coordinate system defined in the tangent plane of the surface at the material point of interest. For $\varphi = 0$, one obtains the micro-free boundary in Eq. (66); while for $\varphi \to \infty$ the micro-clamped boundary condition in Eq. (65) is obtained. One, therefore, obtains the total strain energy stored at the interface in terms of the non-locality residual $\mathbb{R}$ as follows:

$$\int_{\partial\Gamma} \varphi \,\mathrm{d}A = \int_{\partial\Gamma} \left[\int_0^{\boldsymbol{\varepsilon}^{\mathrm{p}(s)}} \tilde{m}_{ij}(\boldsymbol{\varepsilon}^{\mathrm{p}(s)}) \,\mathrm{d}\varepsilon_{ij}^{\mathrm{p}} \right] \mathrm{d}A = \int_{\Gamma} \left[\int_0^t \mathbb{R} \,\mathrm{d}t \right] \mathrm{d}V \geqslant 0 \tag{68}$$

where the fact that the surface stress $\tilde{\mathbf{m}}$ is a function of the surface plastic strain, $\boldsymbol{\varepsilon}^{\mathrm{p}(S)}$, is explicitly indicated. The surface energy is positive definite. Moreover, if $\mathbb{R}$ is neglected, as it is the case for most of current gradient plasticity theories, then the surface energy at interfaces is also neglected. For a given material surface, φ can be measured experimentally or computed using atomistic simulations (e.g. Diao et al., 2004). The interface contributions to the thermodynamic quantities $\tilde{\mathbf{m}}$ and φ are obtained as the excess over the classical thermodynamic values that would be obtained if the strain gradients are absent. It should be mentioned that an elegant mathematical theory incorporating surface stress and interfacial energy into the continuum mechanics formulation was proposed in the 1970s by Gurtin (e.g. Gurtin and Murdoch, 1978; Gurtin et al., 1998).

In case of free surfaces, the higher-order gradient theories (e.g. Fleck and Hutchinson, 2001; Gurtin, 2004; Gudmundson, 2004) assume that the microtraction force $\tilde{\mathbf{m}}$ vanishes analogous to vanishing macrotraction $\mathbf{t}$ at free surfaces. However, like interfaces, free surfaces can also be characterized by a surface energy per unit area. Therefore, another possible interpretation of $\tilde{\mathbf{m}}$ could be the consideration of initial higher-order surface stresses at free surfaces (i.e. $\tilde{\mathbf{m}} = \tilde{\mathbf{m}}_o$) which could exist even when the surface plastic strain $\boldsymbol{\varepsilon}^{\mathrm{p}(S)}$ is absent. These higher-order stresses could be more dominant in structures with high surface-to-volume aspect ratios as in the case of nanosystems. Atomistic simulations show that free surfaces could induce lattice distortion in nanosystems (e.g. Diao et al., 2004). Han et al. (2006) performed discrete dislocation dynamics simulations and found out that free surfaces induce size effects. Furthermore, free surfaces in nanosystems can be sources for development of defects and its propagation towards the interior because of the existence of those higher-order stresses. Therefore, non-vanishing gradients could be encountered at free surfaces even if no prescribed macroscopic tractions $\mathbf{t}$ are imposed at these surfaces. Free surfaces of a material confined in a small volume can strongly affect the size-dependent plasticity. Therefore, imposing non-vanishing microtraction boundary conditions at the free surfaces could result in a size effect under uniaxial loading. The expression for the microtraction stress $\tilde{\mathbf{m}}$ in Eq. (67) can then be modified to incorporate surface and/or interface energies as follows:

$$\tilde{m}_{ij} = \tilde{m}_{ij_0} + \frac{\partial\varphi(\varepsilon^{\mathrm{p}})}{\partial^{(s)}\varepsilon_{ij}^{\mathrm{p}}} \quad \text{on } \partial\Gamma^{\mathrm{p}} \tag{69}$$

where φ can be interpreted now as the energy density of a free surface or an interface (surface/interfacial energy) and is distinct from the bulk deformation-dependent energy. $\tilde{m}_{ij_0} = \tau_o\delta_{ij}$ is the initial surface stress with τ_o representing the deformation-independent surface tension. Therefore, $\tilde{\mathbf{m}}$ can be interpreted as the surface tension at free boundaries. The presence of τ_o could cause the material to deform plastically before the appli-

cation of macroscopic forces. The effect of τ_o has not been incorporated in the formulation of Gudmundson (2004).

3.5. Non-local state variables

The hardening in plasticity is introduced as hidden independent internal state variables in the thermodynamic state potential. The Helmholtz free energy is considered as the thermodynamic state potential depending on both *observable* and *internal* state variables. However, before giving its definition, a choice must be made with respect to the nature of the state variables. Here, one chooses a form of this potential that depends on local and non-local state variables: (a) local variables are the elastic strain, $\boldsymbol{\varepsilon}^{\mathrm{e}}$, the plastic strain, $\boldsymbol{\varepsilon}^{\mathrm{p}}$, and the effective plastic strain p; (b) non-local variables are the plastic strain gradient $\nabla\boldsymbol{\varepsilon}^{\mathrm{p}}$ and the gradient of the effective plastic strain ∇p such that the Helmholtz free energy can be a function of:

$$\Psi = \hat{\Psi}(\varepsilon^{\mathrm{e}}_{ij}, \varepsilon^{\mathrm{p}}_{ij}, p, \varepsilon^{\mathrm{p}}_{ij,k}, p_{,k}) \tag{70}$$

Therefore, to the present authors opinion, the non-local variables $\nabla\boldsymbol{\varepsilon}^{\mathrm{p}}$ and ∇p must appear in the specific free energy Ψ if they do contribute to the internal power expression, Eq. (31).

Assuming a separable material, i.e. no coupling between the elastic and plastic free energies (Gurtin, 2003), one can rewrite the Helmholtz free energy potential as

$$\Psi = \Psi^{\mathrm{e}}(\varepsilon^{\mathrm{e}}_{ij}) + \Psi^{\mathrm{p}}(\varepsilon^{\mathrm{p}}_{ij}, p, \varepsilon^{\mathrm{p}}_{ij,k}, p_{,k}) \tag{71}$$

Taking the time derivative of Eq. (71) with respect to its internal state variables yields

$$\dot{\Psi} = \frac{\partial \Psi^{\mathrm{e}}}{\partial \varepsilon^{\mathrm{e}}_{ij}}\dot{\varepsilon}^{\mathrm{e}}_{ij} + \frac{\partial \Psi^{\mathrm{p}}}{\partial \varepsilon^{\mathrm{p}}_{ij}}\dot{\varepsilon}^{\mathrm{p}}_{ij} + \frac{\partial \Psi^{\mathrm{p}}}{\partial P}\dot{p} + \frac{\partial \Psi^{\mathrm{p}}}{\partial \varepsilon^{\mathrm{p}}_{ij,k}}\dot{\varepsilon}^{\mathrm{p}}_{ij,k} + \frac{\partial \Psi^{\mathrm{p}}}{\partial p_{,k}}\dot{p}_{,k} \tag{72}$$

Making use of Eqs. $(24)_3$ and (25) in Eq. (72), one gets

$$\dot{\Psi} = \frac{\partial \Psi^{\mathrm{e}}}{\partial \varepsilon^{\mathrm{e}}_{ij}}\dot{\varepsilon}^{\mathrm{e}}_{ij} + \left(\frac{\partial \Psi^{\mathrm{p}}}{\partial \varepsilon^{\mathrm{p}}_{ij}} + \frac{\partial \Psi^{\mathrm{p}}}{\partial p}N_{ij}\right)\dot{\varepsilon}^{\mathrm{p}}_{ij} + \left[\frac{\partial \Psi^{\mathrm{p}}}{\partial \varepsilon^{\mathrm{p}}_{ij,k}} + \frac{\partial \Psi^{\mathrm{p}}}{\partial p_{,k}}N_{ij}\right]\dot{\varepsilon}^{\mathrm{p}}_{ij,k} \tag{73}$$

One can now apply the non-local Clausius–Duhem inequality from Eqs. (62) and (60) to the present case along with the expanded time derivative in Eq. (73) such that

$$\left(\sigma_{ij} - \rho\frac{\partial \Psi^{\mathrm{e}}}{\partial \varepsilon^{\mathrm{e}}_{ij}}\right)\dot{\varepsilon}^{\mathrm{e}}_{ij} + \left(\tau_{ij} - \rho\frac{\partial \Psi^{\mathrm{p}}}{\partial \varepsilon^{\mathrm{p}}_{ij}} - \rho\frac{\partial \Psi^{\mathrm{p}}}{\partial p}N_{ij}\right)\dot{\varepsilon}^{\mathrm{p}}_{ij} - \left[\rho\frac{\partial \Psi^{\mathrm{p}}}{\partial \varepsilon^{\mathrm{p}}_{ij,k}} + \rho\frac{\partial \Psi^{\mathrm{p}}}{\partial p_{,k}}N_{ij}\right]\dot{\varepsilon}^{\mathrm{p}}_{ij,k} + \mathbb{R} \geqslant 0 \tag{74}$$

A classical hypothesis permits one to cancel some terms in this inequality independently from which the following thermodynamic state laws are obtained

$$\sigma_{ij} = \rho\frac{\partial \Psi^{\mathrm{e}}}{\partial \varepsilon^{\mathrm{e}}_{ij}} \tag{75}$$

$$J_{ij} = \tau_{ij} - \rho\frac{\partial \Psi^{\mathrm{p}}}{\partial \varepsilon^{\mathrm{p}}_{ij}} - \rho\frac{\partial \Psi^{\mathrm{p}}}{\partial p}N_{ij} \tag{76}$$

$$\mathbb{Z}_{ijk} = -\rho\frac{\partial \Psi^{\mathrm{p}}}{\partial \varepsilon^{\mathrm{p}}_{ij,k}} + \rho\frac{\partial \Psi^{\mathrm{p}}}{\partial p_{,k}}N_{ij} \tag{77}$$

One can also define the local conjugate forces $\mathbf{X}$ and R as

$$X_{ij} = \rho\frac{\partial \Psi^{\mathrm{p}}}{\partial \varepsilon^{\mathrm{p}}_{ij}},\ R = \gamma + \rho\frac{\partial \Psi^{\mathrm{p}}}{\partial p} \tag{78}$$

and the non-local conjugate forces $\mathbf{S}$ and $\mathbf{Q}$ as

$$S_{ijk} = \rho\frac{\partial \Psi}{\partial \varepsilon^{\mathrm{p}}_{ij,k}},\ Q_k = \rho\frac{\partial \Psi}{\partial p_{,k}} \tag{79}$$

It is worthy to mention that from Eq. (78)$_2$ it appears that the isotropic hardening function R is the sum of a dissipative term $\gamma > 0$ and an energetic (or conservative) term $\rho\partial\Psi/\partial p$. The conjugate force R has a hardening or softening effect as $\rho\partial\Psi/\partial p > 0$ or <0, respectively. Moreover, the dissipation modulus γ implicitly incorporates local dissipative effects from R and $\mathbf{X}$ and non-local dissipative effects from $\mathbf{S}$ and $\mathbf{Q}$, which are summed under R. This is shown next.

By substituting Eqs. (78) into Eq. (76), one obtains

$$J_{ij} = \underbrace{\tau_{ij} - X_{ij} - RN_{ij}}_{\text{local microforce balance}} + \gamma N_{ij} \tag{80}$$

However, in the absence of strain gradients, the non-local microforce balance, Eq. (45), reduces to

$$(\tau_{ij} - X_{ij}) - RN_{ij} = 0 \Longleftrightarrow \|\tau_{ij} - X_{ij}\| - R = 0 \tag{81}$$

where Eq. (81)$_2$ defines the local yield surface. Therefore, Eq. (80) can be rewritten as

$$J_{ij} = \gamma N_{ij} \Longleftrightarrow \|J_{ij}\| = \gamma \tag{82}$$

where Eq. (82)$_1$ implies that $\mathbf{N}$ is collinear with $\mathbf{J}$ for local plasticity such that γ is a local quantity in this case. Substituting Eqs. (81)$_2$ and (82)$_2$ into Eq. (82)$_1$ along with Eq. (23)$_2$, one obtains the local plastic flow rule in the absence of strain gradients as follows:

$$\dot{\varepsilon}^{\mathrm{p}}_{ij} = \dot{p}\frac{J_{ij}}{\|J_{ij}\|} \tag{83}$$

or equivalently from Eq. (81)$_1$ as

$$\dot{\varepsilon}^{\mathrm{p}}_{ij} = \dot{p}\frac{\tau_{ij} - X_{ij}}{R} \tag{84}$$

The above equation agrees well with the normality flow rule of classical plasticity.

3.6. Non-local plastic flow rule

By substituting Eqs. (79) into Eq. (77), one obtains Eq. (59). Furthermore, substituting Eqs. (75)–(77) into Eq. (74) reduces the non-local Clausius–Duhem inequality as follows:

$$\Pi = J_{ij}\dot{\varepsilon}^{\mathrm{p}}_{ij} - \mathbb{Z}_{ijk}\dot{\varepsilon}^{\mathrm{p}}_{ij,k} + \mathbb{R} \geqslant 0 \tag{85}$$

where Π is the non-local dissipation energy per unit volume.

By making use of $\mathbb{R}$, Eq. (60), into Eq. (85), one can express Π in a linear form in terms of the driving flux $\dot{\boldsymbol{\varepsilon}}^{\mathrm{p}}$, such that

$$\Pi = \widehat{J}_{ij}\dot{\varepsilon}^{\mathrm{p}}_{ij} \geqslant 0 \tag{86}$$

where $\widehat{\mathbf{J}}$ denotes the unknown total quasi-non-local thermodynamic force and is obtained as

$$\widehat{J}_{ij} = J_{ij} + \mathbb{Z}_{ijk,k} \quad \text{in } \Gamma^{\mathrm{p}} \tag{87}$$

where $\mathbb{R}$ has disappeared from Π in Eq. (85), but its non-locality has been replaced by div $\mathbb{Z}$. Moreover, Eq. (86) proves that the Onsager reciprocity principle (Malvern, 1969) can be assumed to hold in the case of non-local material behavior (Eringen and Edelen, 1972; Polizzotto and Borino, 1998). In the absence of strain gradients, $\widehat{\mathbf{J}}$ degenerates to its local part $\mathbf{J}$. Hence, it is obvious that Eq. (87), after substituting Eqs. (76) and (77), identifies $\widehat{\mathbf{J}}$ and, therefore, it is the force that must be introduced into the non-local evolution equations as the pertinent hardening/softening driving force. $\widehat{\mathbf{J}}$ is a quasi-non-local force since it is decomposed into a local part, $\mathbf{J}$, and a non-local part, div $\mathbb{Z}$.

By substituting Eqs. (76)–(79) into Eq. (87), one can write

$$\hat{J}_{ij} = \underbrace{\tau_{ij} - X_{ij} + S_{ijk,k} - (R - Q_{k,k})N_{ij}}_{\text{non-local microforce balance}} + \gamma N_{ij} \tag{88}$$

Substituting the non-local microforce balance from, Eq. (45), into Eq. (88) yields

$$\hat{J}_{ij} = \gamma N_{ij} \Longleftrightarrow \left\|\hat{J}_{ij}\right\| = \gamma \tag{89}$$

where $\mathbf{N}$ is collinear with $\widehat{\mathbf{J}}$ such that γ is a non-local quantity in this case. Therefore, one can express the plastic flow direction $\mathbf{N}$ form Eqs. (89) and (87) in terms of the quasi-non-local conjugate force $\widehat{\mathbf{J}}$ as follows:

$$N_{ij} = \frac{\widehat{J}_{ij}}{\|\widehat{J}_{mn}\|} = \frac{J_{ij} + \mathbb{Z}_{ijk,k}}{\|J_{mn} + \mathbb{Z}_{mnp,p}\|} \tag{90}$$

This means that the plastic flow is governed by the quasi-non-local force $\widehat{\mathbf{J}}$. By substituting Eqs. (76) and (77) into the above expression, then one obtains the non-local flow rule in Eq. (50). 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 ∇p, while the center of the yield surface (backstress) depends on the plastic strain gradient $\nabla\boldsymbol{\varepsilon}^{\mathrm{p}}$.

Substituting the expression for $\dot{\boldsymbol{\varepsilon}}^{\mathrm{p}}$ from Eq. $(24)_3$ along with Eqs. (89) into Eq. (86) gives

$$\gamma = \frac{\Pi}{\dot{p}} \geqslant 0 \quad \text{for } \dot{p} > 0 \tag{91}$$

where γ is interpreted, according to the notion of Gurtin (2000), as the *non-local dissipation modulus*. Further, one obtains $\gamma = 0$ for $\dot{p} = 0$.

3.7. The non-local maximum dissipation principle

The principle of maximum plastic dissipation (or maximum entropy production) states that the actual state of the thermodynamic forces is that which maximizes the dissipation function over all other possible admissible states (or the closed system should approach its final state of maximal entropy on the shortest possible path). This principle is central in the mathematical formulation of plasticity theories (see e.g. Duvaut and Lions, 1972).

As one observes from the previous discussion, the thermodynamic potential Ψ 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. Eq. (86) expresses the plastic dissipation density, Π, through the local evolution of $\dot{\boldsymbol{\varepsilon}}^{\mathrm{p}}$ and the related non-local thermodynamic force $\widehat{\mathbf{J}}$. Therefore, in case of associative plasticity, as it is the case here, a consistent way to establish the plastic evolution laws is by making use of the maximum plastic dissipation principle. In this regard the evolution laws for $\dot{\boldsymbol{\varepsilon}}^{\mathrm{p}}, \dot{p}, \nabla\boldsymbol{\varepsilon}^{\mathrm{p}}$, and ∇p can be obtained by utilizing the calculus of function of several variables with the Lagrange multiplier, $\dot{\lambda}$, and subjected to the microscopic force balance $f = 0$ from Eq. (49). Formulating this principle, the objective function Ω can be constructed in the following form:

$$\Omega = -\Pi + \dot{\lambda} f \tag{92}$$

The following conditions are used to maximize the objective function, Ω:

$$\frac{\partial \Omega}{\partial \hat{J}_{ij}} = 0 \;\Rightarrow\; \frac{\partial \Omega}{\partial \sigma_{ij}} = 0, \quad \frac{\partial \Omega}{\partial X_{ij}} = 0, \quad \frac{\partial \Omega}{\partial S_{ijk,k}} = 0, \quad \frac{\partial \Omega}{\partial R} = 0, \quad \frac{\partial \Omega}{\partial Q_{kk}} = 0 \tag{93}$$

By making use of Eq. (86) into Eq. (92) along with Eqs. (59), (76), (78) and (87), the plastic flow rule, $\dot{\boldsymbol{\varepsilon}}^{\mathrm{p}}$, can then be obtained from any of the conditions in Eqs. $(93)_{1-4}$, such that

$$\dot{\varepsilon}^{\mathrm{p}}_{ij} = \dot{\lambda}\frac{\partial f}{\partial \hat{J}_{ij}} \Rightarrow = \dot{\varepsilon}^{\mathrm{p}}_{ij} = \dot{\lambda}\frac{\partial f}{\partial \sigma_{ij}} = -\dot{\lambda}\frac{\partial f}{\partial X_{ij}} = \dot{\lambda}\frac{\partial f}{\partial S_{ij,k}} \tag{94}$$

which agrees with the classical assumption that the plastic flow direction $\mathbf{N}$ is governed by the Cauchy stress $\boldsymbol{\sigma}$. However, Eq. (94) suggests that similarly $\mathbf{N}$ is governed by the non-local microstress $\mathrm{div}\mathbf{S}$ as presented in Eq. (55).

The evolution of $\dot{p}$ can be obtained from the last two expressions in Eq. (93) along with Eq. (49) such that

$$\dot{p} = -\dot{\lambda}\frac{\partial f}{\partial R} = \dot{\lambda}\frac{\partial f}{\partial Q_{k,k}} = \dot{\lambda} \tag{95}$$

where $\dot{\lambda}$ is the plastic multiplier which can be determined by the non-local consistency condition

$$f \leqslant 0, \quad \dot{\lambda} \geqslant 0, \quad \dot{\lambda} f = 0 \quad \text{and} \quad \dot{\lambda}\dot{f} = 0 \tag{96}$$

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 Ψ and its identification from experiments. Several examples are presented in the following section.

It is noteworthy that Gurtin and Anand (2005) and Anand et al. (2005) have argued that in order to be able to capture *strengthening* and the increase in rates of *strain hardening* accompanied by the reduction in size, one should adopt two material length scales: *dissipative* and *energetic* length scales, respectively. The energetic length scale is associated with the gradient of plastic strain tensor, $\nabla\boldsymbol{\varepsilon}^{\mathrm{p}}$, whereas the dissipative length scale is associated with the gradient of the effective plastic strain, ∇p. However, in Gurtin's analysis ∇p does not directly enter the definition of the internal virtual power but as a constitutive assumption through a power-law (see Section 6 of Gurtin and Anand, 2005). Therefore, the current formulation differs from Gurtin's work in that both $\nabla\boldsymbol{\varepsilon}^{\mathrm{p}}$ and ∇p along with their local counterparts, $\boldsymbol{\varepsilon}^{\mathrm{p}}$ and p, enter the definitions of the internal virtual power, Eq. (31). By doing so the non-local form of the von-Mises yield criterion is obtained directly from the principle of virtual power without further constitutive assumptions as shown in Section 3.2. Therefore, by setting $R = Q_{k,k} = 0$ in the current derived microscopic force balance, Eq. (45), and adopting the same constitutive relations for the microstresses $\mathbf{X}$ and $\mathbf{S}$ as presented in Gurtin and Anand (2005) and Anand et al. (2005) one obtains the exact expressions for the microforce balance and the non-local plastic flow rule as derived by Gurtin. Moreover, the proposed model differs from Gurtin's analysis in that definite values for the microscopic boundary conditions are obtained depending on the level of surface/interface energy, whereas null microscopic boundary conditions are assumed in the work of Gurtin, which are very difficult to be satisfied in practice. Finally, the current thermodynamic framework preserves the classical structure of local plasticity theory. This is not inline with 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 $\boldsymbol{\sigma}$. The proposed framework suggests that $\mathbf{N}$ is governed by $\boldsymbol{\sigma}$ or equivalently by $\mathrm{div}\mathbf{S}$.

4. Gradient-dependence of the Helmholtz free energy

In order to develop equations amenable to the analysis and computation, one now considers examples for the definition of the Helmholtz free energy function.

Example 1. One can assume decoupling between the elastic behavior and plasticity hardening (i.e. separable material) such that both Ψ^{e} and Ψ^{p} that appear in Eq. (71) can be assumed to have, respectively, the following quadratic analytical form:

$$\rho\Psi^{\mathrm{e}} = \frac{1}{2}\varepsilon^{\mathrm{e}}_{ij}E_{ijkl}\varepsilon^{\mathrm{e}}_{kl} \tag{97}$$

$$\rho\Psi^{\mathrm{p}} = \frac{1}{2}a_1\varepsilon^{\mathrm{p}}_{ij}\varepsilon^{\mathrm{p}}_{ij} + \frac{1}{2}a_2p^2 + \frac{1}{2}a_3\varepsilon^{\mathrm{p}}_{ij,k}\varepsilon^{\mathrm{p}}_{ij,k} + \frac{1}{2}a_4p_{,k}p_{,k} \tag{98}$$

where $\mathbf{E}$ is the symmetric fourth-order elastic stiffness tensor and $a_i (i = 1\text{-}4)$ are material constants.

Now, one can obtain the Cauchy stress from Eqs. (75) and (97) as

$$\sigma_{ij} = E_{ijkl}\varepsilon^{\mathrm{e}}_{kl} = E_{ijkl}(\varepsilon_{kl} - \varepsilon^{\mathrm{p}}_{kl}) \tag{99}$$

Making use of Eqs. $(23)_2$ and $(25)_2$, the local and non-local conjugate forces in Eqs. (78) and (79) can be obtained, respectively, as follows:

$$X_{ij} = h\varepsilon^{\mathrm{p}}_{ij}, \qquad R = \gamma + hp \tag{100}$$

$$S_{ijk} = B_{ijmn}\varepsilon^{\mathrm{p}}_{mn,k}, \qquad Q_k = hl^2 p_{,k} \tag{101}$$

where, for simplicity, it is assumed that $a_1 + a_2 = h$ and $a_3 + a_4 = h\ell^2$ with h being the constant hardening modulus, $B_{ijmn} = a_3\delta_{im}\delta_{jn} + a_4 N_{ij}N_{mn}$, and $\gamma = \sigma_{\mathrm{y}}$ coincides with the initial yield strength.

Substituting Eqs. (100) and (101) into the yield function f, Eq. (49), one can then write

$$f = \underbrace{\|\tau_{ij} + X_{ij} + S_{ijk,k}\|}_{\text{effective Von-Mises stress}} - \underbrace{\gamma - hp + h\ell^2\nabla^2 p}_{\text{isotropic hardening function}} = 0 \tag{102}$$

with

$$S_{ijk,k} = B_{ijmn,k}\varepsilon^{\mathrm{p}}_{mn,k} + B_{ijmn}\varepsilon^{\mathrm{p}}_{mn,kk} \tag{103}$$

where ∇^2 designates the Laplacian operator and $B_{ijmn,k} = a_4\,(N_{ij,k}N_{mn} + N_{ij}N_{mn,k})$.

Thus this theory shows that the Laplacian of the effective plastic strain contributes to the size of the yield surface (isotropic hardening), whereas the first-order gradient and the Laplacian of the plastic strain tensor contribute 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 $\nabla\boldsymbol{\varepsilon}^{\mathrm{p}}$ and the effective plastic strain ∇p and, respectively, not to $\nabla^2\boldsymbol{\varepsilon}^{\mathrm{p}}$ and $\nabla^2 p$, consistent with basic notions of the role of the net Burgers vector and the geometrically necessary dislocations. Instead, $\nabla^2\boldsymbol{\varepsilon}^{\mathrm{p}}$ and $\nabla^2 p$ emerges in the resulting field equations as a byproduct of the more fundamental role of the plastic strain gradients.

Example 2. More complicated non-local yield functions can be obtained if one assumes non-quadratic or anisotropic analytical expressions in the definition of the Helmholtz free energy function, Eq. (98). For example, the invariant $a_3\boldsymbol{\varepsilon}^{\mathrm{p}}_{ij,k}\boldsymbol{\varepsilon}^{\mathrm{p}}_{ij,k}$ in Eq. (98) can be replaced by one or some of the following quadratic invariants (Gurtin, 2003):

$$\rho\Psi^{\mathrm{p}}(\varepsilon^{\mathrm{p}}_{ij,k}) = \frac{1}{2}c_1\varepsilon^{\mathrm{p}}_{ij,k}\varepsilon^{\mathrm{p}}_{ij,k} + \frac{1}{2}c_2\varepsilon^{\mathrm{p}}_{ij,k}\varepsilon^{\mathrm{p}}_{ik,j} + \frac{1}{2}c_3\varepsilon^{\mathrm{p}}_{ij,j}\varepsilon^{\mathrm{p}}_{ik,k} \tag{104}$$

where $\boldsymbol{\varepsilon}^{\mathrm{p}}_{ij,k}\boldsymbol{\varepsilon}^{\mathrm{p}}_{ij,k} = \|\nabla\boldsymbol{\varepsilon}^{\mathrm{p}}\|^2, \|\nabla\boldsymbol{\varepsilon}^{\mathrm{p}}\|^2 - \boldsymbol{\varepsilon}^{\mathrm{p}}_{ij,k}\boldsymbol{\varepsilon}^{\mathrm{p}}_{ik,j} = \|\mathrm{curl}\boldsymbol{\varepsilon}^{\mathrm{p}}\|^2$, and $\boldsymbol{\varepsilon}^{\mathrm{p}}_{ij,j}\boldsymbol{\varepsilon}^{\mathrm{p}}_{ik,k} = \|\mathrm{div}\,\boldsymbol{\varepsilon}^{\mathrm{p}}\|^2$ such that $\boldsymbol{\varepsilon}^{\mathrm{p}}_{ij} = \boldsymbol{\varepsilon}^{\mathrm{p}}_{ji}$ and $\boldsymbol{\varepsilon}^{\mathrm{p}}_{kk} = 0$. Substituting the above expression into Eq. $(79)_1$ yields a complicated expression for the conjugate force $\mathbf{S}$ as

$$S_{ijk} = c_1\varepsilon^{\mathrm{p}}_{ij,k} + \frac{1}{2}c_2(\varepsilon^{\mathrm{p}}_{kj,j} + \varepsilon^{\mathrm{p}}_{ki,j}) + \frac{1}{2}c_3(\varepsilon^{\mathrm{p}}_{im,m}\delta_{jk} + \varepsilon^{\mathrm{p}}_{jm,m}\delta_{ik}) - \frac{1}{3}(c_2 + c_3)\varepsilon^{\mathrm{p}}_{km,m}\delta_{ij} \tag{105}$$

such that one can express $\mathrm{div}\,\mathbf{S}$ as

$$S_{ijk,k} = c_1\varepsilon^{\mathrm{p}}_{ij} + (c_2 + c_3)\left(\frac{\varepsilon^{\mathrm{p}}_{ik,kj} + \varepsilon^{\mathrm{p}}_{jk,ki}}{2} - \frac{\varepsilon^{\mathrm{p}}_{mk,km}\delta_{ij}}{3}\right) \tag{106}$$

Example 3. The plasticity related component of the Helmholtz free energy can be expressed in terms of the plastic strain gradient $\nabla\boldsymbol{\varepsilon}^{\mathrm{p}}$ by adopting the Fleck and Hutchinson (2001) decompositions of $\nabla\boldsymbol{\varepsilon}^{\mathrm{p}}$ into three orthogonal components

$$\varepsilon^{\mathrm{p}}_{ij,k} = \sum_{m=1}^{3}\varepsilon^{\mathrm{p}(m)}_{ij,k} \tag{107}$$

with

$$\varepsilon^{\mathrm{p}(1)}_{ij,k} = \varepsilon^{\mathrm{p}(s)}_{ijk} - \frac{1}{5}(\delta_{ij}\varepsilon^{\mathrm{p}(s)}_{kp,p} + \delta_{ik}\varepsilon^{\mathrm{p}(s)}_{jp,p} + \delta_{jk}\varepsilon^{\mathrm{p}(s)}_{ip,p}) \tag{108}$$

$$\varepsilon^{\mathrm{p}(2)}_{ij,k} = \frac{1}{6}\left[(e_{ikp}e_{jlm} + e_{jkp}e_{ilm})\varepsilon^{\mathrm{p}}_{lp,m} + 2\varepsilon^{\mathrm{p}}_{ij,k} - \varepsilon^{\mathrm{p}}_{jk,i} - \varepsilon^{\mathrm{p}}_{ki,j}\right] \tag{109}$$

$$\varepsilon^{\mathrm{p}(3)}_{ij,k} = \frac{1}{6}\left[(e_{ikp}e_{jlm}\varepsilon^{\mathrm{p}}_{lp,m} + e_{jkp}e_{ilm})\varepsilon^{\mathrm{p}}_{lp,m} + 2\varepsilon^{\mathrm{p}}_{ij,k} - \varepsilon^{\mathrm{p}}_{jk,i} - \varepsilon^{\mathrm{p}}_{ki,j}\right] + \frac{1}{5}(\delta_{ij}\varepsilon^{\mathrm{p}(s)}_{kp,p} + \delta_{ik}\varepsilon^{\mathrm{p}(s)}_{jp,p} + \delta_{jk}\varepsilon^{\mathrm{p}(s)}_{ip,p}) \tag{110}$$

where δ_{ij} is the Kronecker delta, e_{ijk} is the permutation tensor, and $\boldsymbol{\varepsilon}^{\mathrm{p}(s)}_{ij,k}$ is the fully symmetric part of $\boldsymbol{\varepsilon}^{\mathrm{p}}_{ij,k}$,

$$\varepsilon^{\mathrm{p}(s)}_{ij,k} = \frac{1}{3}(\varepsilon^{\mathrm{p}}_{ij,k} + \varepsilon^{\mathrm{p}}_{jk,i} + \varepsilon^{\mathrm{p}}_{ki,j}) \tag{111}$$

Therefore, a free energy that depends on an isotropic and quadratic form in the plastic strain gradients may be expressed as follows (Gudmundson, 2004):

$$\rho\Psi^{\mathrm{p}}(\varepsilon^{\mathrm{p}}_{ij,k}) = \frac{1}{2}\sum_{m=1}^{3} c^{(m)}\varepsilon^{\mathrm{p}(m)}_{ij,k}\varepsilon^{\mathrm{p}(m)}_{ij,k} \tag{112}$$

Substituting the above expression into Eq. $(79)_1$ yields the following expression for the conjugate force $\mathbf{S}$

$$S_{ijk} = \sum_{m=1}^{3} c^{(m)}\varepsilon^{\mathrm{p}(m)}_{ij,k} \tag{113}$$

such that one can express $\mathrm{div}\mathbf{S}$ as

$$S_{ijk,k} = \sum_{m=1}^{3} c^{(m)}\varepsilon^{\mathrm{p}(m)}_{ij,kk} \tag{114}$$

Example 4. For general power-law constitutive relations, one can assume the traditional power-law for the defect free energy, Ψ^{p}, such that:

$$\rho\Psi^{\mathrm{p}}(E^{\mathrm{p}}) = \frac{h}{m+2}\left(\frac{E^{\mathrm{p}}}{\varepsilon_{\mathrm{y}}}\right)^{m+2}\varepsilon^2_{\mathrm{y}} \tag{115}$$

where $m > 0$ is the rate-sensitivity parameter, E^{p} is the non-local effective plastic strain presented in Eq. (29), and $\boldsymbol{\varepsilon}_{\mathrm{y}}$ is the yield strain. The isotopic hardening conjugate forces can be obtained by making use of Eqs. $(78)_2$ and $(79)_2$, respectively, as follows:

$$R = \gamma + h\left(\frac{E^{\mathrm{p}}}{\varepsilon_{\mathrm{y}}}\right)^{m} p, \qquad Q_k = h\ell^2\left(\frac{E^{\mathrm{p}}}{\varepsilon_{\mathrm{y}}}\right)^{m} p,k \tag{116}$$

From the above expressions one can express the yield criterion in Eq. (49) as follows:

$$f = \|\tau_{ij} - X_{ij} + S_{ijk,k}\| - \gamma - h\left(\frac{E^{\mathrm{p}}}{\varepsilon_{\mathrm{y}}}\right)^{m} p + h\ell^2\frac{\partial}{\partial x_k}\left[\left(\frac{E^{\mathrm{p}}}{\varepsilon_{\mathrm{y}}}\right)^{m} p_{,k}\right] = 0 \tag{117}$$

which coincides with the expression proposed by Gurtin and Anand (2005) where $\mathrm{div}\mathbf{S}$ is given either by Eq. (106) or Eq. (114). It can be noticed that the limit $m \to 0$ gives Eq. (102).

It is noteworthy that in Gurtin and Anand (2005) and Anand et al. (2005) the higher-order stress $\mathbf{S}$ conjugate to $\nabla\boldsymbol{\varepsilon}^{\mathrm{p}}$ is split into an energetic part, $\mathbf{S}_{\mathrm{en}}$, and a dissipative part, $\mathbf{S}_{\mathrm{dis}}$, such that

$$\mathbf{S} = \mathbf{S}_{\mathrm{en}} + \mathbf{S}_{\mathrm{dis}}$$

Therefore, by setting $R = Q_{k,k} = 0$ in the current derived microscopic force balance, Eq. (45), one obtains the exact form for the microforce balance as derived by Gurtin, such that:

$$\boldsymbol{\tau} + \mathrm{div}\mathbf{S}_{\mathrm{en}} = \mathbf{X} - \mathrm{div}\mathbf{S}_{\mathrm{dis}}$$

However, in order to obtain viscoplastic constitutive model, the following constitutive relations for the micro-stresses, $\mathbf{X}$, $\mathbf{S}_{\mathrm{en}}$, and $\mathbf{S}_{\mathrm{dis}}$, have been assumed by Gurtin and Anand (2005) and Anand et al. (2005):

$$\mathbf{X} = h\left(\frac{\dot{E}^{\mathrm{p}}}{\dot{\varepsilon}_{\mathrm{y}}}\right)^{m}\frac{\dot{\boldsymbol{\varepsilon}}^{\mathrm{p}}}{\dot{E}^{\mathrm{p}}}, \mathbf{S}_{\mathrm{dis}} = \ell^2 h\left(\frac{\dot{E}^{\mathrm{p}}}{\dot{\boldsymbol{\varepsilon}}_{\mathrm{y}}}\right)^{m}\frac{\nabla\dot{\boldsymbol{\varepsilon}}^{\mathrm{p}}}{\dot{E}^{\mathrm{p}}}$$

with $\mathbf{S}_{\mathrm{en}} = \rho\frac{\partial\Psi^{\mathrm{p}}(\nabla\boldsymbol{\varepsilon}^{\mathrm{p}})}{\partial\nabla\boldsymbol{\varepsilon}^{\mathrm{p}}}$, which yields the same expression as in Eq. (105). Therefore, substituting these relations in the microscopic force balance yields the same expression for the plastic flow as presented in Gurtin and Anand (2005) and Anand et al. (2005). In other words, one can obtain Gurtin's formulation by neglecting the effective plastic strain, p, and the corresponding gradient, ∇p, in the current model, or equivalently by setting the corresponding conjugate forces q, R, and Q_k zero in the definitions of the external and internal virtual powers in Eqs. (30) and (31), respectively. Furthermore, the specific forms for the plastic flow rule and plastic dissipation as presented in Gurtin and Anand (2005) and Anand et al. (2005) can be obtained easily by adopting their constitutive assumptions for the defect energy and the isotropic hardening function. Therefore, both Gurtin's analysis and the analysis presented in this work are overall equivalent when ∇p and p are neglected.

As presented in Section 3.4, additional boundary conditions have to be specified on the elastic-plastic interface for plastic strains or higher-order stresses. Constrained plastic flow could be modeled either as a full constraint, i.e. $\boldsymbol{\varepsilon}^{\mathrm{p}} = 0$, as in Eq. (65) or no constraint, i.e. $\tilde{\mathbf{m}} = 0$, as in Eq. (66). However, following the ideas presented by Gudmundson (2004), an intermediate kind of micro-boundary condition is introduced. Therefore, the surface energy φ presented in Eq. (67) that depends on the plastic strain state at the interface can be assumed to have the following quadratic form:

$$\varphi = \frac{1}{2}h\ell_{\mathrm{S}}\varepsilon_{ij}^{\mathrm{p}(s)}\varepsilon_{ij}^{\mathrm{p}(s)} \quad \text{on } \partial\Gamma^{\mathrm{p}} \tag{118}$$

where ℓ_{S} is a microstructural length scale that is related to boundary layer thickness and characterizes the strength of the surface/interface boundary. The microtraction stress at the boundary, $\tilde{\mathbf{m}}$, can then be obtained from Eqs. (67) and (118) as

$$\tilde{m}_{ij} = \tilde{m}_{ij0} + h\ell_{\mathrm{S}}\varepsilon_{ij}^{\mathrm{p}(s)} \quad \text{on } \partial\Gamma^{\mathrm{p}} \tag{119}$$

The microtraction stress is thus collinear with the plastic strain at the interface. If $\ell_{\mathrm{S}} = 0$ and $\tilde{\mathbf{m}}_0 = 0$, the interface would behave like a free surface and one obtains the micro-free boundary condition, Eq. (66). On the other hand, if $\ell_{\mathrm{S}} \to \infty$ then it would represent a condition for fully constrained dislocation movement at the interface and one obtains the micro-clamped boundary condition, Eq. (65). The role of the deformation-independent surface stress $\tilde{m}_{ij_o} = \tau_o\delta_{ij}$ on the predictions of size effects will be investigated in future work.

5. Applications to size effects in thin films

This section presents some recent applications of gradient plasticity to handle size effects observed in metals. The proposed gradient plasticity theory is now used to investigate the size dependent behavior in biaxial loading of a plastic thin film on an elastic substrate, shear loading of a thin film fixed to a rigid substrate, and thermal cooling of a thin film on a substrate. In the following applications, for simplicity, kinematic hardening introduced by the conjugate forces $\mathbf{X}$ and $\mathbf{S}$ is neglected and the expression of the yield surface f in Eq. (102) is employed.

5.1. 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 Fig. 1. Let x_3 be the perpendicular axis to the film and $x_3 = 0$ corresponds to the film–substrate interface. The loading is defined by a monotonically increasing biaxial strain ε_0 such that $\varepsilon_{11} = \varepsilon_{22} = \varepsilon_0$. A plane stress situation is assumed such that the non-vanishing stress components are

$$\sigma_{11} = \sigma_{22} = \sigma_0(x_3) \tag{120}$$

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

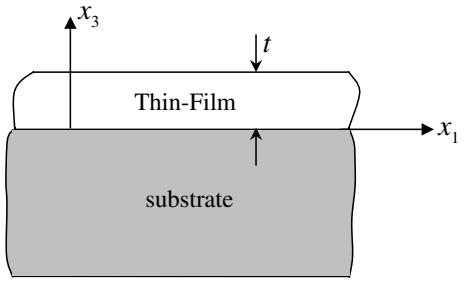

Fig. 1. An elasto-plastic thin film of thickness t on elastic substrate.

$$\varepsilon^{\mathrm{p}}_{11} = \varepsilon^{\mathrm{p}}_{22} = -\frac{1}{2}\varepsilon^{\mathrm{p}}_{33} = \varepsilon^{\mathrm{p}}_{0}(x_3) \tag{121}$$

The effective plastic strain $p = \sqrt{\boldsymbol{\varepsilon}^{\mathrm{p}}_{ij}\boldsymbol{\varepsilon}^{\mathrm{p}}_{ij}}$ and its Laplacian $\nabla^2 p$ are given as

$$p = \sqrt{6}\varepsilon^{\mathrm{p}}_{0} \quad \text{and} \quad \nabla^2 p = \sqrt{6}\varepsilon^{\mathrm{p}}_{0,33} \tag{122}$$

where $\boldsymbol{\varepsilon}^{\mathrm{p}}_{o,33} = \partial\boldsymbol{\varepsilon}^{\mathrm{p}}_{o}/\partial x_3\partial x_3$.

The stress–strain relationship can be simply obtained from the generalized Hook's law as

$$\sigma_0(x_3) = \frac{E}{(1-\nu)}(\varepsilon_0 - \varepsilon^{\mathrm{p}}_{0}(x_3)) \tag{123}$$

Substituting Eqs. (120), (122) and (123) into the yield condition, Eq. (102), yields the following ordinary differential equation for $\boldsymbol{\varepsilon}^{\mathrm{p}}_{o}(x_3)$:

$$\varepsilon^{\mathrm{p}}_{o,33} - \left[\frac{1}{\ell^2} + \frac{E}{3(1-\nu)h\ell^2}\right]\varepsilon^{\mathrm{p}}_{o} = \frac{\sigma_{\mathrm{y}}}{\sqrt{6}h\ell^2} - \frac{E}{3(1-\nu)h\ell^2}\varepsilon_o \tag{124}$$

It is convenient to express the above equation in a non-dimensional form with the aid of variable substitution (i.e. $z = x_3/t, \bar{\boldsymbol{\varepsilon}}^{\mathrm{p}}_{o} = \boldsymbol{\varepsilon}^{\mathrm{p}}_{o}/\varepsilon_{\mathrm{y}}$, and $\bar{\varepsilon}_o = \varepsilon_o/\varepsilon_{\mathrm{y}}$ with $\varepsilon_{\mathrm{y}} = (1-\nu)\sigma_{\mathrm{y}}/E$ being the in-plane yield strain) such that

$$\bar{\varepsilon}^{\mathrm{p}}_{o,zz} - \lambda^2\bar{\varepsilon}^{\mathrm{p}}_{o} = -F \tag{125}$$

with constant coefficients λ and F are given through

$$\lambda^2 = \frac{1}{(\ell/t)^2}\left(1 + \frac{E}{3(1-\nu)h}\right) \quad \text{and} \quad F = \frac{E(\bar{\varepsilon}_o - \sqrt{3/2})}{3(1-\nu)h(\ell/t)^2} \tag{126}$$

The micro-boundary conditions can now be utilized as presented by Eq. (119). The microtraction stress $\tilde{\mathbf{m}}$ can be obtained from Eqs. (46) to $(101)_2$ as

$$\tilde{m}_{11} = \tilde{m}_{22} = -\frac{1}{2}\tilde{m}_{33} = h\ell^2\varepsilon^{\mathrm{p}}_{o,3} \tag{127}$$

It is assumed that the microtraction stress $\tilde{\mathbf{m}}$ vanishes at the free surface ($x_3 = t$) such that Eq. (127) results in the following microfree boundary condition

$$\frac{\partial\bar{\varepsilon}^{\mathrm{p}}_{o}}{\partial z} = 0 \quad \text{at } z = 1 \tag{128}$$

The boundary condition at the film–substrate interface is given from Eqs. (119) to (127) as follows:

$$(\ell_{\mathrm{S}}/\ell)\bar{\varepsilon}^{\mathrm{p}}_{o} = (\ell/t)\frac{\partial\bar{\varepsilon}^{\mathrm{p}}_{o}}{\partial z} \ \textit{at } z = 0 \tag{129}$$

Solving the ordinary differential equation, Eq. (125), which is subjected to the boundary conditions in Eqs. (128) and (129), one obtains a closed-form expression for $\bar{\boldsymbol{\varepsilon}}^{\mathrm{p}}_{o}(z)$ as

$$\bar{\varepsilon}_o^{\mathrm{p}}(Z) = \frac{F}{\lambda^2}\left[1 - \frac{\cosh\lambda(1-z)}{\cosh\lambda + \delta\sinh\lambda}\right] \tag{130}$$

where F/λ^2 and δ are given by

$$\frac{F}{\lambda^2} = \frac{E(\bar{\varepsilon}_o - \sqrt{3/2})}{3(1-\nu)h + E} H(\bar{\varepsilon}_o - \sqrt{3/2}) \tag{131}$$

$$\delta^2 = \lambda^2(\ell/t)^2(\ell/\ell_{\mathrm{S}})^2 = (\ell/\ell_{\mathrm{S}})^2\left(1 + \frac{E}{3(1-\nu)h}\right) \tag{132}$$

where $H(\bar{\varepsilon}_o - \sqrt{3/2})$ is the Heaviside step function.

For $\delta = 0$, which corresponds to the micro-clamped boundary condition at the film–substrate interface as presented in Eqs. (65), (130) reduces to

$$\bar{\varepsilon}_o^{\mathrm{p}}(z) = \frac{F}{\lambda^2}[1 - \cosh\lambda Z + \tanh\lambda\sinh\lambda Z] \tag{133}$$

Substituting Eq. (130) back into the normalized expression of Eq. (123) (i.e. the in-plane stresses are normalized by the yield stress σ_{y} such that $\bar{\sigma}_o = \bar{\varepsilon}_o - \bar{\varepsilon}_o^{\mathrm{p}}$), one finds the following:

$$\bar{\sigma}_o = \bar{\varepsilon}_o - \frac{E(\bar{\varepsilon}_o - \sqrt{3/2})}{3(1-\nu)h + E}\left[1 - \frac{\cosh\lambda(1-z)}{\cosh\lambda + \delta\sinh\lambda}\right] H(\bar{\varepsilon}_o - \sqrt{3/2}) \tag{134}$$

The average stress in the thin-film, $\bar{\sigma}_o^{\mathrm{ave}}$, can be determined from an integration of Eq. (134) from 0 to 1, such that:

$$\bar{\sigma}_o^{\mathrm{ave}} = \bar{\varepsilon}_o - \frac{E(\bar{\varepsilon}_o - \sqrt{3/2})}{3(1-\nu)h + E}\left[1 - \frac{\tanh\lambda}{\lambda(1 + \delta\tanh\lambda)}\right] H(\bar{\varepsilon}_o - \sqrt{3/2}) \tag{135}$$

Results in Figs. 2–4 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, and 2. The level of surface energy in the film–substrate interface is controlled by the ratio ℓ_{S}/ℓ. Results are presented for $\ell_{\mathrm{S}}/\ell = 1$, 10, and ∞ corresponding to soft, intermediate, and hard interfaces, respectively.

In Figs. 2–4(a), normalized results for average film stress, Eq. (135), vs. applied biaxial strain ε_o are presented. It is clearly seen that the hardening tangent modulus and the film stress increase with decreasing the film thickness, which agree qualitatively with the experimental observations. However, this increase is smaller for soft interface than for intermediate and hard interfaces. Therefore, one anticipates that no size effect should be encountered as ℓ_{S}/ℓ goes to zero (i.e. the interface represents a free surface). The size effect for hard interface is strongly pronounced. Similar trends have been obtained by Anand et al. (2005) and Fredriksson and Gudmundson (2005). They have also shown that the initial yield stress increases with increasing ℓ/t for hard interfaces (i.e. $\ell_{\mathrm{S}}/\ell \to \infty$). This sort of increase can be obtained by using their constitutive assumptions for the gradient-dependent Helmholtz free energy, such that the yield condition, Eq. (102), can be expressed as follows:

$$f = \|\tau_{ij} - X_{ij} + S_{ijk,k}\| - \sigma_{\mathrm{y}}\left(1 + \frac{E^{\mathrm{p}}}{\varepsilon_{\mathrm{y}}}\right)^m + h\ell^2\nabla^2 p = 0 \tag{136}$$

where σ_{y} is the coarse grain yield strength, E^{p} is the generalized effective plastic strain given in Eq. (29), and $0 < m < 1$. For simplicity, the above yield function is not used because the aforementioned closed form solutions can not be obtained and a finite element implementation becomes necessary. This will be presented in future work.

Figs. 2–4(b) and (c) show the variation of the biaxial stress and plastic strain, Eqs. (134) and (130), 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. However, this increase or decrease depends on the level of surface energy at the interface. The higher is the surface energy (implied by higher ℓ_{S}/ℓ) the less plastic deformation is allowed at the

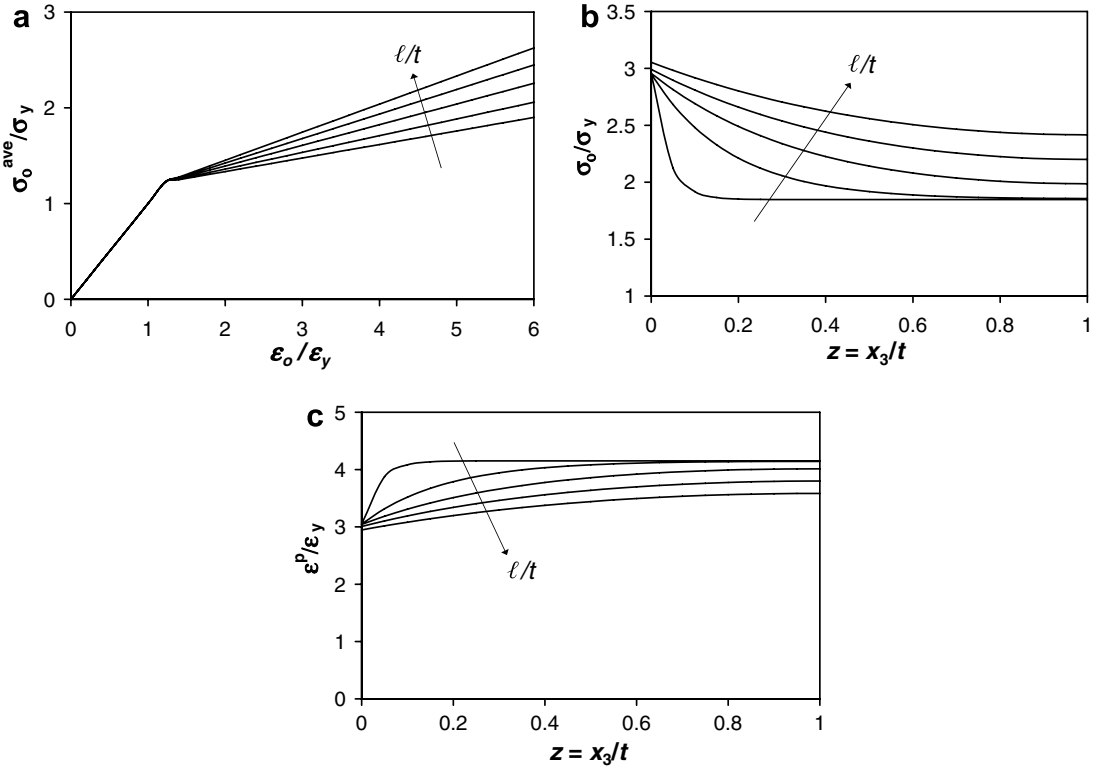

Fig. 2. Biaxial tension for a soft interface; $\ell_S/\ell = 1$. Different film thicknesses are represented by $\ell/t = 0.1, 0.5, 1, 1.5, 2$ for: (a) average biaxial stress vs. biaxial strain, (b) biaxial stress through the thickness at a strain of $\varepsilon_o = 6\varepsilon_y$, and (c) biaxial plastic strain through the thickness.

interface, which results in a higher biaxial stress. For the hard interface, the biaxial stress at the interface is equal to the elastic stress, $\sigma_o = 6\sigma_y$, i.e. the plastic strain is equal to zero.

Moreover, due to the constraint placed on the plastic strain, a boundary layer of thickness t/λ develops through the film thickness. Interestingly, the thickness of the boundary layer is independent of the biaxial strain ε_o and does not vary with time, but scales with ℓ. For example, $\ell/t = 0.5$ implies a boundary layer of thickness $0.18t$ that only occupies a part of the film close to the interface, while $\ell/t = 2$ occupies almost the entire film, $0.9t$. This type of behavior applies to all values of ℓ_S/ℓ as shown in Figs. 2–4(b) and (c). Moreover, the results clearly show that the biaxial stress and plastic strain profiles tend to become homogeneous with increased thickness and decrease surface energy due to smaller gradient effects. This means that gradients eventually disappear for large thicknesses and small surface energies. As shown in Figs. 2–4(c), the increase of plastic strain at $z = 1$ (free surface) overwhelms the increase of the plastic strain gradient due to the distribution of gradients such that gradients decrease as the free boundary is approached and increase as the substrate is approached. Therefore, the elimination of gradients spreads from the free boundary, propagating through the entire thickness. Finally, the plastic strain becomes uniform across the thickness.

As the surface energy is increased, the reduced plastic strain in the boundary layer is compensated by higher elastic strains, thus leading to higher stresses. Therefore, the results in Fig. 5 show that the hard interface reveals a pronounced size effect as compared to the soft and intermediate interfaces.

5.2. 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 Fig. 1. Therefore, the bottom surface of the film is held fixed and a shear traction τ_0 is applied to the top surface in the x_1-

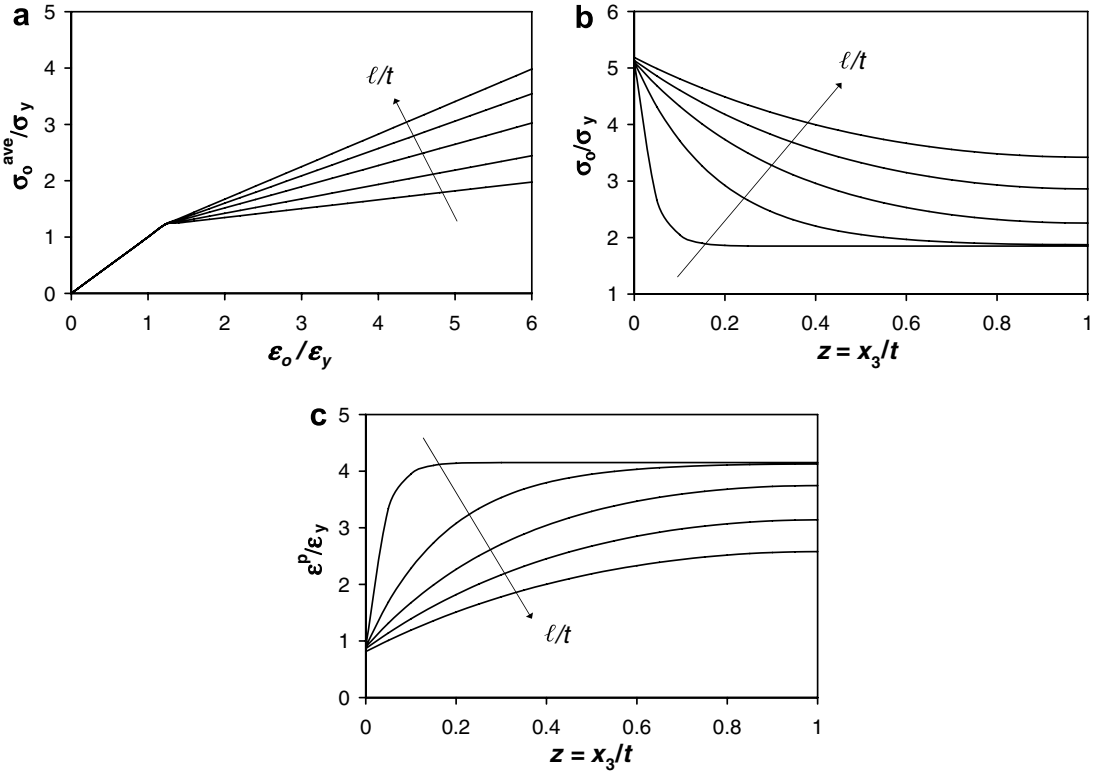

Fig. 3. Biaxial tension for an intermediate interface; $\ell_S/\ell = 10$. Different film thicknesses are represented by $\ell/t = 0.1, 0.5, 1, 1.5, 2$ for: (a) average biaxial stress vs. biaxial strain, (b) biaxial stress through the thickness at a strain of $\varepsilon_o = 6\varepsilon_y$, and (c) biaxial plastic strain through the thickness.

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. Shu et al. (2001) have 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

$$\sigma_{31} = \tau_o, \quad \varepsilon^p_{31} = \frac{1}{2}\gamma^p_o(x_3) \tag{137}$$

where τ_0 is homogeneous across the film thickness since the macroscopic force balance, Eq. (43), yields $\partial\tau_0/\partial x_3 = 0$ if the body forces and inertia are neglected.

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

$$p = \frac{1}{2}\gamma^p_o(x_3) \quad \text{and} \quad \nabla^2 p = \frac{1}{2}\gamma^p_{o,33} \tag{138}$$

where $\gamma^p_{0,33} = \partial\gamma^p_0/\partial x_3\partial x_3$. The stress–strain relationship is given by Hook's law as

$$\tau_o = G\big(\gamma_o - \gamma^p_o(x_3)\big) \tag{139}$$

where G is the elastic shear modulus. Substituting Eqs. (137) and (138) into the yield condition, Eq. (102), yields the following ordinary differential equation for $\gamma^p_0(x_3)$:

$$\gamma^p_{0,33} - \frac{1}{\ell^2}\gamma^p_o = -\frac{2}{h\ell^2}(\tau_o\sqrt{3}\tau_y) \tag{140}$$

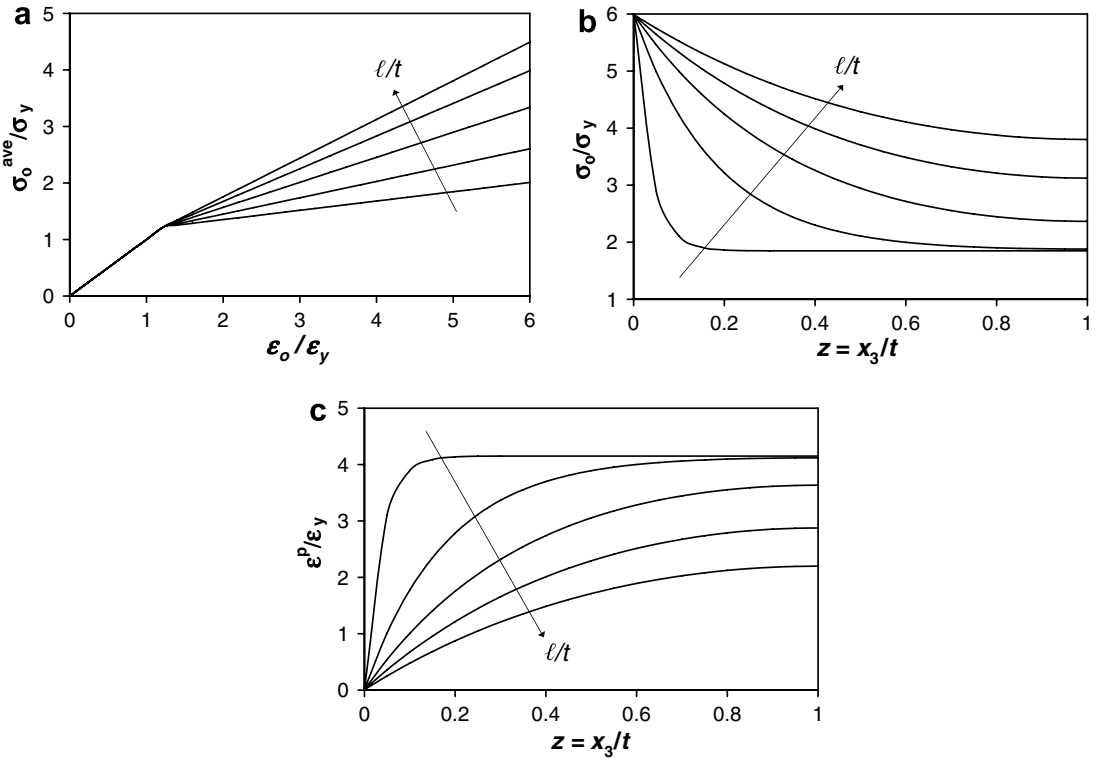

Fig. 4. Biaxial tension for a hard interface; $\ell_S/\ell \to \infty$. Different film thicknesses are represented by $\ell/t = 0.1, 0.5, 1, 1.5, 2$ for: (a) average biaxial stress vs. biaxial strain, (b) biaxial stress through the thickness at a strain of $\varepsilon_o = 6\varepsilon_y$, and (c) biaxial plastic strain through the thickness.

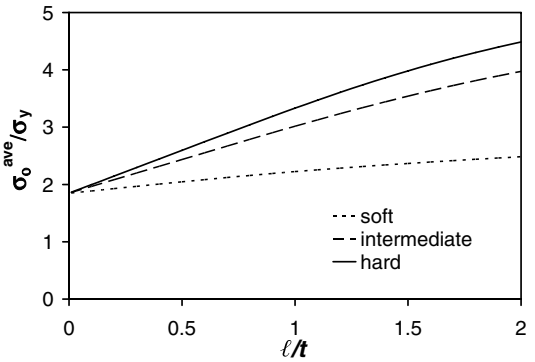

Fig. 5. Biaxial tension for soft,intermediate,and hard interfaces. Average biaxial stress vs. normalized film thickness.

where τ_y is the shear yield stress. In order to express the above equation in a non-dimensional form, one can proceed completely analogous to biaxial loading in Section 5.1. With the aid of variable substitution (i.e. $z = x_3/t, \bar{\gamma}_0^p = \gamma_0^p/\gamma_y$, and $\bar{\tau}_0 = \tau_0/\tau_y$ with $\gamma_y = \tau_y/G$ being the shear yield strain), Eq. (140) can be written as

$$\bar{\gamma}^p_{o,zz} - \lambda^2 \bar{\gamma}^p_o = -F \tag{141}$$

with constant coefficients λ and F are given by

$$\lambda^2 = \frac{1}{(\ell/t)^2} \quad \text{and} \quad F = \frac{2G(\bar{\tau}_o - \sqrt{3})}{h(\ell/t)^2} \tag{142}$$

Non-uniform plastic strain can be enhanced by applying the micro-boundary conditions presented in Eq. (119). The microtraction-free boundary condition, Eq. (66), is imposed at $x_3 = t$ such that

$$\frac{\partial \bar{\gamma}_o^{\mathrm{p}}}{\partial z} = 0 \quad \text{at } z = 1 \tag{143}$$

The boundary condition at the film–substrate interface is given from Eqs. (119) to (127) as follows:

$$(\ell_{\mathrm{S}}/\ell)\bar{\gamma}_o^{\mathrm{p}} = (\ell/t)\frac{\partial \bar{\gamma}_o^{\mathrm{p}}}{\partial z} \quad \text{at } z = 0 \tag{144}$$

Therefore, it is not necessary to assume an initial non-uniform plastic strain distribution across the film thickness in order to enhance strain gradient evolution.

Solving the ordinary differential equation, Eq. (141), which is subjected to the boundary conditions in Eqs. (143) and (144), one obtains a closed-form expression for $\bar{\gamma}_0^{\mathrm{p}}(z)$ as

$$\bar{\gamma}_o^{\mathrm{p}}(Z) = \frac{F}{\lambda^2}\left[1 - \frac{\cosh\lambda(1-z)}{\cosh\lambda + \gamma\sinh\lambda}\right] \tag{145}$$

with

$$\frac{F}{\lambda^2} = \frac{2G}{h}(\bar{\tau}_o - \sqrt{3})H(\bar{\tau}_o - \sqrt{3}), \quad \delta = \ell/\ell_{\mathrm{S}} \tag{146}$$

where $H(\bar{\tau}_0 - \sqrt{3})$ is the Heaviside step function. Substituting Eq. (145) back into the normalized expression of Eq. (139) (i.e. the shear stress is normalized by the yield stress τ_{y} such that $\bar{\tau}_0 = \bar{\gamma}_0 - \bar{\gamma}_0^{\mathrm{p}}$), one can write the total shear strain as follows:

$$\bar{\gamma}_o(Z) = \bar{\tau}_o + \frac{2G}{h}(\bar{\tau}_o - \sqrt{3})\left[1 - \frac{\cosh\lambda(1-z)}{\cosh\lambda + \delta\sinh\lambda}\right]H(\bar{\tau}_o - \sqrt{3}) \tag{147}$$

It can be noted that the micro-boundary conditions, Eqs. (143) and (144), are crucial for obtaining size effect solutions.

The average shear strain in the thin-film, $\bar{\gamma}_0^{\mathrm{ave}}$, can be determined from an integration of Eq. (147) from 0 to 1, such that:

$$\bar{\gamma}_o^{\mathrm{ave}} = \bar{\tau}_o + \frac{2G}{h}(\bar{\tau}_o - \sqrt{3})\left(1 - \frac{\tanh\lambda}{\lambda(1+\delta\tanh\lambda)}\right)H(\bar{\tau}_o - \sqrt{3}) \tag{148}$$

Results in Figs. 6–8 are presented for $h/G = 0.15$. The surface energy at the interface between the film and the substrate is defined by the parameter δ. Different film thicknesses are captured by different ℓ/t. Different interface properties are also presented here by $\ell_{\mathrm{S}}/\ell = 1, 10$, and ∞.

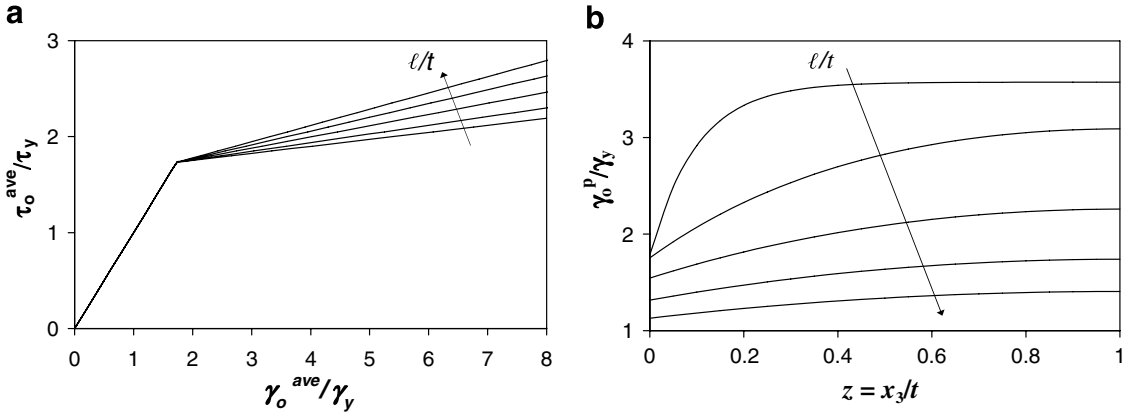

Fig. 6. Pure shear for a soft interface; $\ell_{\mathrm{S}}/\ell = 1$. Different film thicknesses are represented by $\ell/t = 0.1, 0.5, 1, 1.5, 2$ for: (a) shear stress vs. average shear strain, and (b) plastic shear strain across the thickness at an average stress of $\tau_o/\tau_{\mathrm{y}} = 2$.

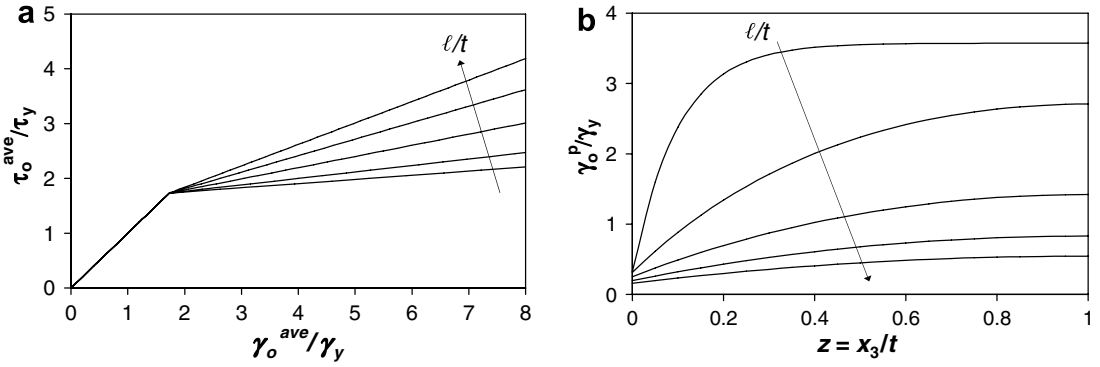

Fig. 7. Pure shear for an intermediate interface; $\ell_S/\ell = 10$. Different film thicknesses are represented by $\ell/t = 0.1, 0.5, 1, 1.5, 2$ for: (a) shear stress vs. average shear strain and (b) plastic shear strain across the thickness at an average stress of $\tau_o/\tau_y = 2$

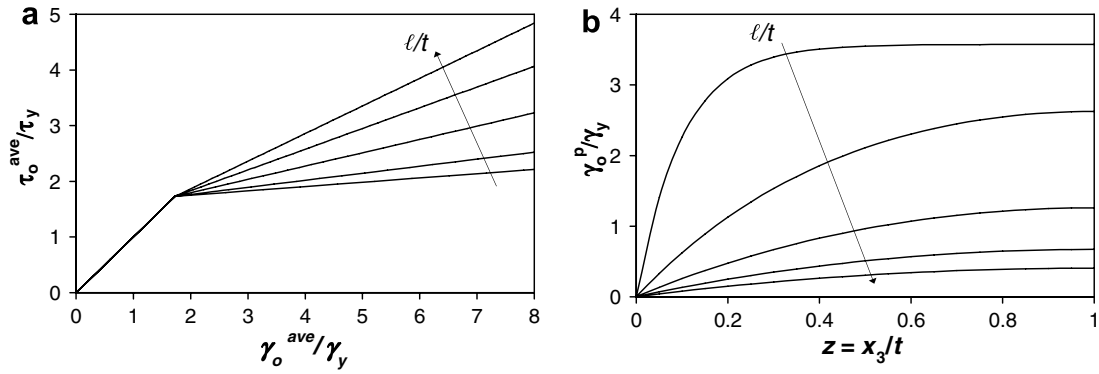

Fig. 8. Pure shear for a hard interface; $\ell_S/\ell \to \infty$. Different film thicknesses are represented by $\ell/t = 0.1, 0.5, 1, 1.5, 2$ for: (a) shear stress vs. average shear strain and (b) plastic shear strain across the thickness at an average stress of $\tau_o/\tau_y = 2$.

Similar results to biaxial loading are obtained. In Fig. 6–8, normalized plots for average film strain, Eq. (148), vs. the normalized applied stress $\bar{\tau}_0$ and the plastic shear strain, Eq. (146), through the film thickness at $\bar{\tau}_0 = 2$ are presented for different ℓ_S/ℓ. Instead of a uniform distribution across the film thickness, the plastic shear strain decreases as the interface is approached due to the constraint. For a thick film, equivalent to $\ell/t \to 0$, the results would coincide with the local plasticity theory solution, which would give homogeneous plastic strain in the film. If $\ell/t \to \infty$ a pure elastic state would be obtained in the film.

Figs. 6–8(a) show that the hardening increases with ℓ/t, particularly, with increasing ℓ_S/t as is also seen for biaxial strain. Moreover, it is shown in Figs. 6–8(b) that ℓ_S/ℓ controls the constraint on γ_0^p at the interface. Furthermore, Figs. 6–8(b) clearly show a boundary layer near the interface, in which the plastic shear strain is reduced in order to meet the microtraction boundary condition, Eq. (144). Inspection of the expression in Eq. (145) reveals that the thickness of this boundary layer is set by the length scale ℓ. For larger values of ℓ the boundary layer thickness is of the same order as the specimen thickness t and the effect of the boundary condition is noticeable even near the free surface (at $x_3/t = 0$). If ℓ is decreased, the boundary layer becomes thinner and the plastic shear strain profile approaches that of the classical plasticity.

5.3. Thermal loading of a thin film on a substrate

The problem of a thin film on a semi-infinite substrate subjected to thermal loading will be studied now. This problem has been investigated by Nicola et al. (2003) using discrete-dislocation dynamics. A quasi-static monotonic thermal loading is imposed by cooling the film–substrate system from an initial temperature T_0, at

which the film and substrate are stress free and dislocation free. The substrate undergoes unconstrained contraction but, due to the mismatch between the thermal-expansion coefficient of the film (α_f) and the substrate (α_S), stress develops in the film; tensile for $\alpha_f > \alpha_S$.

Since the film is infinitely long in the x_1-direction and initially homogeneous, the solution depends only on x_3 such that by assuming a plane strain problem in the x_2-direction one can write

$$\sigma_{33} = \sigma_{13} = 0, \quad \sigma_{11} = \sigma_o(x_3) \tag{149}$$

where the stress field $\sigma_0(x_3)$ is non-uniform and unknown at this stage. Because of symmetry and because the strain components do not depend on $x_1, \dot{\varepsilon}_{11}$ must be uniform throughout the film such that from the plastic incompressibility assumption one can express the non-vanishing plastic strain components in the film as

$$\varepsilon^{\mathrm{p}}_{11} = -\frac{1}{2}\varepsilon^{\mathrm{p}}_{33} = \varepsilon^{\mathrm{p}}_o(x_3) \tag{150}$$

The effective plastic strain $p = \sqrt{\boldsymbol{\varepsilon}^{\mathrm{p}}_{ij}\boldsymbol{\varepsilon}^{\mathrm{p}}_{ij}}$ and its Laplacian are $\nabla^2 p$ given as

$$p = \sqrt{5}\varepsilon^{\mathrm{p}}_o \quad \text{and} \quad \nabla^2 p = \sqrt{5}\varepsilon^{\mathrm{p}}_{o,33} \tag{151}$$

where $\boldsymbol{\varepsilon}^{\mathrm{p}}_{0,33} = \partial\boldsymbol{\varepsilon}^{\mathrm{p}}_0/\partial x_3\partial x_3$. For plane strain condition, the stress–strain rate relationship can be expressed as follows:

$$\dot{\sigma}_{11}(x_3) = \frac{E}{1-\nu^2}\dot{\varepsilon}^{\mathrm{e}}_{11}(x_3) \tag{152}$$

The rate of the total strain in the film is decomposed into an elastic part, a plastic part, and a thermal part given by

$$\dot{\varepsilon}_{11} = \dot{\varepsilon}^{\mathrm{e}}_{11} + \dot{\varepsilon}^{\mathrm{p}}_{11} + (1+\nu)\alpha_{\mathrm{f}}\dot{T} \tag{153}$$

The total strain rate in the elastic substrate is given by

$$\dot{\varepsilon}_{11} = (1+\nu)\alpha_{\mathrm{S}}\dot{T} \tag{154}$$

where compatibility of deformation between the film and the substrate requires that $\dot{\varepsilon}_{11}$ be the same and uniform throughout the film. Hence, substituting Eqs. (153) and (154) into Eq. (152) along with the time derivative of Eqs. $(149)_2$ and (150) yields

$$\dot{\sigma}_o(x_3) = \frac{E}{1-\nu^2}[(1+\nu)(\alpha_{\mathrm{S}} - \alpha_{\mathrm{f}})\dot{T} - \dot{\varepsilon}^{\mathrm{p}}_o(x_3)] \tag{155}$$

One can express the consistency condition from the yield condition in Eq. (102) as

$$\dot{f} = \frac{1}{3}\dot{\sigma}_o - h\dot{\varepsilon}^{\mathrm{p}}_o + h\ell^2\dot{\varepsilon}^{\mathrm{p}}_{o,33} = 0 \tag{156}$$

Substituting Eq. (155) into Eq. (156), yields the following ordinary differential equation for $\dot{\boldsymbol{\varepsilon}}^{\mathrm{p}}_0(x_3)$:

$$\dot{\varepsilon}^{\mathrm{p}}_{o,33} - \left[\frac{1}{\ell^2} + \frac{E}{3(1-\nu)h\ell^2}\right]\dot{\varepsilon}^{\mathrm{p}}_o = -\frac{E}{3(1-\nu)h\ell^2}(\alpha_{\mathrm{S}} - \alpha_{\mathrm{f}})\dot{T} \tag{157}$$

It is convenient to express the above equation in a non-dimensional form with the aid of variable substitution (i.e. $z = x_3/t$) such that

$$\dot{\varepsilon}^{\mathrm{p}}_{o,zz} - \lambda^2\dot{\varepsilon}^{\mathrm{p}}_o = -\dot{F} \tag{158}$$

with constant coefficients λ and $\dot{F}$ given through

$$\lambda^2 = \frac{1}{(\ell/t)^2}\left(1 + \frac{E}{3(1-\nu^2)h}\right) \quad \text{and} \quad \dot{F} = \frac{E(\alpha_{\mathrm{S}} - \alpha_{\mathrm{f}})\dot{T}}{3(1-\nu)h(\ell/t)^2} \tag{159}$$

Now the null micro-boundary conditions as presented by Eqs. (66) and (65) are examined. The microtraction-free boundary condition at the film top (i.e. $x_3 = t$), where dislocations can freely leave the film, and the micro-

plastic-clamped boundary condition at the film–substrate interface, where slip cannot occur, such that one can write, respectively, the following:

$$\frac{\partial \varepsilon_o^{\mathrm{p}}}{\partial z} = 0 \text{ at } z = 1 \quad \text{and} \quad \varepsilon_o^{\mathrm{p}} = 0 \text{ at } z = 0 \tag{160}$$

Solving the ordinary differential equation, Eq. (158), which is subjected to the boundary conditions in Eqs. (160), one obtains a closed-form expression for $\dot{\boldsymbol{\varepsilon}}_0^{\mathrm{p}}(z)$ as

$$\dot{\varepsilon}_o^{\mathrm{p}}(z) = \frac{\dot{F}}{\lambda^2}(1 - \cosh \lambda z + \tanh \lambda \ \sinh \lambda z) \tag{161}$$

where

$$\frac{\dot{F}}{\lambda^2} = \frac{E(1+\nu)(\alpha_{\mathrm{S}} - \alpha_{\mathrm{f}})\dot{T}}{3(1-\nu^2)h + E} \tag{162}$$

In the elastic range, one can integrate Eq. (155) from zero to the onset of yield (at $\sigma_0 = \gamma$ and at temperature $T_{\mathrm{y}} < T_0$) by setting $\dot{\boldsymbol{\varepsilon}}_0^{\mathrm{p}} = 0$, such that the following expression can be obtained for $\gamma = \sigma_{\mathrm{y}}$ in terms of T_{y}:

$$\sigma_{\mathrm{y}} = -\frac{E}{1-\nu}(\alpha_{\mathrm{f}} - \alpha_{\mathrm{S}})(T_{\mathrm{y}} - T_o) \tag{163}$$

where σ_{y} is the uniform film stress at the onset of yield (at yield temperature T_{y}). Moreover, substituting Eqs. (161) and (162) back into Eq. (155), one finds a linear relation between $\dot{\sigma}_0$ and $\dot{T}$ given by

$$\dot{\sigma}_o(z) = \frac{E}{1-\nu^2}\left[(1+\nu) - \frac{E(1+\nu)}{3(1-\nu^2)h + E}(1 - \cosh \lambda z + \tanh \lambda \sinh \lambda z)\right](\alpha_{\mathrm{S}} - \alpha_{\mathrm{f}})\dot{T} \tag{164}$$

In the plastic range, one can integrate Eqs. (161) and (164) from the onset of yield to the current stress σ_0 and temperature T such that one gets, respectively,

$$\varepsilon_o^{\mathrm{p}}(z) = \frac{(1-\nu^2)c}{E}(1 - \cosh \lambda z + \tanh \lambda \sinh \lambda z) \tag{165}$$

and

$$\sigma_o(z) = \sigma_n + c(1 - \cosh \lambda z + \tanh \lambda \sinh \lambda z) \tag{166}$$

where σ_n and c are given by

$$\sigma_n = -\frac{E}{1-\nu}(\alpha_{\mathrm{f}} - \alpha_{\mathrm{S}})(T - T_o), \quad c = \frac{E^2(\alpha_{\mathrm{f}} - \alpha_{\mathrm{S}})(T - T_{\mathrm{y}})}{(1-\nu)[3(1-\nu^2)h + E]} \tag{167}$$

Here σ_n is the stress in the absence of plasticity; for $T = T_Y$ one retains Eq. (163).

The average stress in the thin-film, σ_0^{ave}, can be determined from an integration of Eq. (166), such that:

$$\sigma_o^{\mathrm{ave}} = \sigma_n + c\left(1 - \frac{\tanh \lambda}{\lambda}\right) \tag{168}$$

Results in Fig. 9 are presented for straining of an aluminum film on a silicon substrate during thermal loading. Typical properties of aluminum are adopted ($E = 70$ GPa, $\nu = 0.33$, $\alpha_{\mathrm{f}} = 23.2 \times 10^{-6}$/K, $\sigma_{\mathrm{y}} = 36$ MPa, and $h = 100$ MPa). The silicon coefficient of thermal expansion is taken to be $\alpha_S = 23.2 \times 10^{-6}$/K. Results are obtained by cooling the film–substrate system from an initial temperature at $T_0 = 600$ K to $T = 400$ K. The temperature at which yielding occurs is obtained from Eq. (163) to be $T_{\mathrm{y}} = 582$ K. Different film thicknesses are represented by $\ell/t = 0.1, 0.5, 1, 1.5$, and 2. Very similar qualitative results to that presented in Fig. 4 are obtained. The results in Fig. 9(a) show that the average in-plane stress, Eq. (168), and the integral of Eq. (154), in the film is strongly dependent on the film thickness. The stress is normalized by the elastic stress σ_n, Eq. $(167)_1$. Fig. 9(b) shows the average stress-temperature curves given by Eqs. (167) and (168), which reinforces the strong size effect. Moreover, the linear hardening is consistent with the discrete dislocation simulations obtained by Nicola et al. (2003). Fig. 9(c) and (d) show the variation of the stress and plastic strain, Eqs.

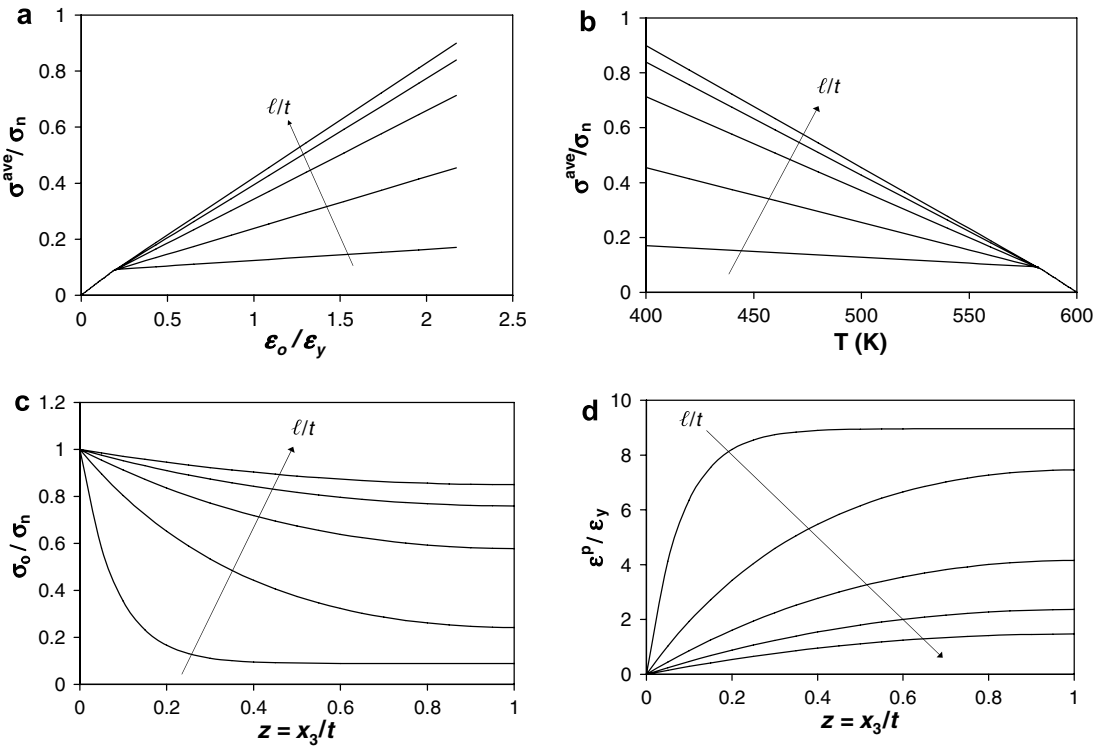

Fig. 9. Thermal cooling of an aluminum-silicon thin film–substrate system by 200K. Different film thicknesses are represented by $\ell/t = 0.1, 0.5, 1, 1.5, 2$ for: (a) average stress vs.strain, (b) average stress and temperature, (c) stress through the thickness, and (d) plastic strain through the thickness.

(166) and (165), across the film thickness. The stress increases and the plastic strain decreases as the film–substrate interface is approached. These results are in good agreement with the discrete dislocation simulations by Nicola et al. (2003).

6. Concluding remarks

Gradient-dependent variational and thermodynamic framework is presented in this paper that extends the classical plasticity to higher-order gradient plasticity theory. Higher-order stresses and higher-order boundary conditions are formulated in a unified way. It is shown that a non-local form of the Clausius–Duhem inequality should be used in deriving gradient-dependent constitutive equations. As compared to the classical Clausius–Duhem inequality an additional term that accounts for the non-local interactions at interfaces and free surfaces appears in the non-local Clausius–Duhem inequality.

Moreover, the proposed framework is a two non-local parameter theory that takes into account large variations in the plastic strain tensor and large variations in the accumulated (effective) plastic strain. It is argued that the gradient of the plastic strain tensor, $\boldsymbol{\varepsilon}^{p}_{ij,k}$, and the gradient of the effective plastic strain, $p_{,k}$, should be incorporated when formulating a gradient plasticity theory since the former accounts for the Nye's dislocation density (or incompatibility) tensor and the later accounts for the accumulation of the geometrically necessary dislocations. The thermodynamic conjugate force associated with $\boldsymbol{\varepsilon}^{p}_{ij,k}$ introduces kinematic hardening whereas the conjugate force of $p_{,k}$ introduces isotropic hardening.

The formulation of higher-order boundary conditions is very important within strain gradient plasticity theory, especially, at interfaces, grain, or phase boundaries. A framework for the formulation of these additional boundary conditions is presented. The microlevel significance and nature of these boundary conditions is emphasized. It is shown for certain problems (e.g. biaxial loading of a film–substrate system, shear loading

of a constrained layer, or thermal loading of film–substrate system), in which the material is initially homogenous, that in the absence of the higher-order boundary conditions, the material would support uniform fields and hence the constitutive gradient-dependence would have no influence. Therefore, strain gradients come into play if the boundaries are assumed to constrain the plastic flow. This constraint is set by the level of surface/interface energy. Hence, this is a central part for 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. These examples have shown that the present theory can qualitatively describe many features of the size effect, including development of boundary layers and the strain hardening. In the present examples of a thin film–substrate system, the substrate is assumed to be soft, intermediate, or hard depending on the level of interface energy where dislocations in the film are partially or completely blocked as they approach the film–substrate interface. The results show a strong dependence on the interface energy. A larger energy results in a more pronounced size effect. Moreover, dislocations approaching a free surface could be free to pass out and producing unconstrained plastic strain, which results in vanishing plastic strain gradients at the free surface. However, dislocations could pileup partially at a free surface depending on the magnitude of the microtraction stress which increases as the surface-to-volume ratio increases; therefore, non-vanishing local gradients in plastic strain could be encountered at the free surface. The authors believe that the later effect is crucial for the interpretation of size effects encountered in nano systems. In small confined volumes the microtraction stress could be high enough at the free surfaces which results in a micro-clamped boundary where dislocations tend to pileup leading to the presence of strain gradients. Therefore, the dislocation pileups at interface/free surfaces can be modeled by non-vanishing microtraction stresses, or equivalently, finite expenditure of non-local power.

Similarly to numerous gradient-dependent models, the full utility of the gradient-type theories in bridging the gap between modeling, simulation, and design of modern technology hinges on one's ability to determine accurate values for the constitutive length scale parameter ℓ that scales the effects of strain gradients. The study of Begley and Hutchinson (1998), Nix and Gao (1998), Shu and Fleck (1998), Yuan and Chen (2001), Abu Al-Rub and Voyiadjis (2004a,b), and Voyiadjis and Abu Al-Rub (2004) indicated that indentation experiments might be the most effective test for measuring ℓ. For more details about the physical origin and the measurement of the material length scale ℓ the reader is referred to Abu Al-Rub (2004) and Abu Al-Rub and Voyiadjis (2006, in press).

In conclusion, if continuum theories are to be used to predict elastic-plastic behavior at the micron or submicron length scales, a higher-order theory is likely to be required. Moreover, it would be of particular interest to compare the effects of microtraction stresses at interfaces and free surfaces in the present gradient theory with discrete dislocation dynamics simulations.

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