Modelling size effects in micro/nano-systems by including interfacial effects in a gradient plasticity framework

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Abstract: The effect of the material microstructural interfaces increases as the surface-to-volume ratio increases. It is shown in this work that interfacial effects have a profound impact on the scale-dependent plasticity encountered in micro/nano-systems. This is achieved by developing a physically-based higher-order gradient-dependent plasticity theory that enforces microscopic boundary conditions at interfaces and free surfaces. These non-standard boundary conditions relate the micro traction stress at the interface to the interfacial energy. Application of the proposed framework to size effects in biaxial tension of a thin-film on an elastic substrate is presented. Three film-interface conditions are modelled: soft, intermediate, and hard interfaces.

Keywords: interfacial energy; non-local; size effect; thin films; length scale.

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1 Introduction

The emerging areas of micro- and nano-technologies exhibit important strength differences that result from continuous modification of the material microstructural characteristics with changing size, with smaller being stronger. There are many experimental observations which indicate that, under certain specific conditions, the size of micro/nano-systems significantly affects their strength such that a length scale is required for predicting such size effects when using the classical theories of continuum mechanics. For example, experimental works have shown increase in strength by decreasing:

a the particle size in nano-composites

b the diameter of nano-wires in torsion and uniaxial compression

c the thickness of thin films in micro-bending and uniaxial tension

d the grain size of nano-crystalline materials

e void size in nano-porous media

f the indentation depth in micro/nano indentation tests, etc. [see Abu Al-Rub and Voyiadjis (2004, 2006) for a complete list of references].

Plastic deformation in small scale structures, accommodated by dislocation nucleation and movement, is strongly affected by interfaces. Until now, little attention is devoted to interfacial effects (e.g., film-substrate interface, phase or grain boundaries, inclusion's interface, void free surface, nano-wires free surfaces, etc.) on the scale-dependent plasticity in small scale systems (e.g., thin films, thin wires, nano-composites, etc.). Investigations of interface conditions have recently been presented by Gudmundson (2004), Fredriksson and Gudmundson (2005), Gurtin and Needleman (2005), Aifantis and Willis (2005, 2006) and Abu Al-Rub et al. (2007). Interfaces between distinct regions can be locations for dislocations' blocking and pileups, and hence decreasing plastic flow and increasing the strength. Dislocation pileups, which result in local plastic strain gradients, could be encountered at the interface depending on the level of *interfacial energy* which increases as the surface-to-volume ratio increases. In other words, it is expected that as the specimen size decreases, the higher is the interfacial energy and the more significant is the effect of the boundary layer thickness on the strength.

Size effects in micro/nano-systems could not be explained by the classical continuum mechanics since no length scale enters the constitutive description (Fleck et al., 1994). A multiscale continuum theory, therefore, is needed to bridge the gap between the classical continuum theories and micro mechanical theories. Since the increase in strength with decreasing scale can be related to proportional increase in the strain gradients (Aifantis, 1984), the gradient plasticity theory has been successful in addressing the size effect problem [see Voyiadjis and Abu Al-Rub (2005) for an extensive review of successful examples]. 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. Furthermore, for mathematical consistency, in the gradient-dependent framework, additional boundary conditions have to be specified at interfaces and free surfaces allowing one to include interfacial effects.

It is shown in the present paper that interfacial strengthening effects can be characterised within the strain gradient plasticity theory by incorporating an interfacial energy term in the internal work that depends on the plastic strain state at the interface of the plastically deforming material. Therefore, a physically-based gradient-dependent plasticity theory that complies with dislocation-based mechanics and incorporates interfacial stress and interfacial energy is formulated here based on the principle of virtual power and the non-local Clausius-Duhem inequality. As a result, two material length scales are incorporated: one for the bulk material and one for the interface, which together control the size effect at the micro- and nano-levels.

As an application of the proposed framework, the role of three types of interfaces on strain hardening of a biaxially loaded thin film-substrate system is presented. Depending on the interfacial energy, these three interface conditions are briefly studied:

1 hard interfaces (corresponding to hard substrates), characterised by high interfacial energies, which completely block the dislocation motion and hence constrain the plastic flow

2 compliant interfaces (corresponding to compliant substrates), characterised by moderate interfacial energies, which partially block the dislocation motion and hence plastic flow is increased

3 soft interfaces (corresponding to soft substrates), characterised by low interfacial energies, which significantly decrease dislocation obstruction and pileups.

2 Crystallographic basis for the presence of plastic strain gradients

Small strain/small rotation plasticity and rate-independent material response is assumed here. The classical theory of isotropic plastic solids undergoing small deformations is based on the additive decomposition of the total strain, $\boldsymbol{\varepsilon}$, into an elastic part, $\boldsymbol{\varepsilon}^e$, and a plastic part, $\boldsymbol{\varepsilon}^p$:

$$\varepsilon_{ij} = \varepsilon_{ij}^e + \varepsilon_{ij}^p \tag{1}$$

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

$$\varepsilon_{ij}^p = \sum\nolimits_{\beta} p^{(\beta)} \mu_{ij}^{(\beta)}, \;\; \mu_{ij}^{(\beta)} = \tfrac{1}{2}\left(s_i^{(\beta)} n_j^{(\beta)} + n_i^{(\beta)} s_j^{(\beta)} \right) \tag{2}$$

where $\boldsymbol{\mu}^{(\beta)}$ is the symmetric Schmidt orientation tensor, and $\mathbf{s}^{(\beta)}$ and $\mathbf{n}^{(\beta)}$ are the unit vectors characterising the slip direction on the slip plane β and its normal, respectively, such that $\| \mathbf{s}^{(\beta)} \| = \| \mathbf{n}^{(\beta)} \| = 1$ and $\mathbf{s}^{(\beta)} \cdot \mathbf{n}^{(\beta)} = 0$.

Material deformation in metallic micro- and nano-systems enhances the dislocation nucleation, the dislocation motion, and the dislocation storage within the grain bulk and at the grain boundaries and material interfaces. 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 within the polycrystal caused by non-uniform dislocation slip (i.e., plastic strain gradients) 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 (Ashby, 1970). 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):

$$\alpha_{ij} = \sum\nolimits_{\xi} \rho_G^{(\xi)} b_i^{(\xi)} t_j^{(\xi)} \tag{3}$$

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. The total accumulation of GNDs is

obtained as the magnitude of Nye's dislocation density tensor, $\alpha = \| \boldsymbol{\alpha} \|$, such that if one neglects the interaction among different slip systems, α reads:

$$\alpha = \rho_G b \tag{4}$$

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

For irrotational plastic flow (i.e., neglecting the plastic spin tensor), $\boldsymbol{\alpha}$ can be related to the gradient of plastic strain tensor, $\nabla \boldsymbol{\varepsilon}^p$, by (e.g., Fleck et al., 1994):

$$\alpha_{ij} = e_{jkl} \varepsilon^p_{il,k} \tag{5}$$

where e_{irq} is the permutation symbol. By substituting equation $(2)_1$ into equation (5), $\boldsymbol{\alpha}$ can be written as follows:

$$\alpha_{ij} = \sum\nolimits_\beta p^{(\beta)}_{,k} \eta^{(\beta)}_{ikj} \tag{6}$$

where $\eta^{(\beta)}_{ikj} = e_{jkl} \mu^{(\beta)}_{il}$. Therefore, equation (6) relates the dislocation density tensor to the slip gradients. Equating equations (3) and (6) gives the gradient of plastic strain tensor in terms of GNDs density as:

$$e_{jkl} \varepsilon^p_{il,k} = \sum\nolimits_\xi \rho_G^{(\xi)} b_i^{(\xi)} t_j^{(\xi)} \tag{7}$$

One can define the accumulation of GNDs, α, from equation (6) as follows:

$$\alpha = \sum\nolimits_\beta \sqrt{p^{(\beta)}_{,k} p^{(\beta)}_{,k}} \tag{8}$$

It can be noted that the accumulation of GNDs is related to the magnitude of plastic slip gradients. Equating equations (4) and (8) gives the magnitude of plastic slip gradients in terms of the GNDs density as:

$$\sum\nolimits_\beta \sqrt{p^{(\beta)}_{,k} p^{(\beta)}_{,k}} = \rho_G b \tag{9}$$

which agrees with the relation proposed by Ashby (1970).

3 Thermodynamics of higher-order gradient plasticity

In order to be able to model the small-scale phenomena, such as the effect of size of microstructural features on the material mechanical properties, an attempt is made here to account for the effect of plastic strain gradients on the homogenised response of the material. This is done by developing a higher-order gradient-dependent theory using the principle of virtual power and the laws of thermodynamics. A continuum plasticity theory is developed here. A crystal plasticity theory will be developed in a forthcoming paper.

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

$$\dot{p} = \left\| \dot{\varepsilon}^p_{ij} \right\| = \sqrt{\dot{\varepsilon}^p_{ij} \dot{\varepsilon}^p_{ij}} \tag{10}$$

while the unit direction of plastic strain tensor, **N**, is defined as follows:

$$N_{ij} = \dot{\varepsilon}^p_{ij} \Big/ \| \dot{\varepsilon}^p_{ij} \| = \dot{\varepsilon}^p_{ij} \Big/ \dot{p} \Rightarrow \dot{\varepsilon}^p_{ij} = \dot{p} N_{ij} \Rightarrow \dot{p} = \dot{\varepsilon}^p_{ij} N_{ij} \tag{11}$$

Substituting equation $(2)_1$ into equation (10) and neglecting interactions between different slip planes, yields $\dot{p} = \sum_\beta \dot{p}^{(\beta)}$. One can also write the following useful relation by taking the gradient of equation (10) such that:

$$\dot{p}_{,k} = \frac{\dot{\varepsilon}^p_{ij} \dot{\varepsilon}^p_{ij,k}}{\sqrt{\dot{\varepsilon}^p_{mn} \dot{\varepsilon}^p_{mn}}} = \frac{\dot{\varepsilon}^p_{ij}}{\dot{p}} \dot{\varepsilon}^p_{ij,k} = N_{ij} \dot{\varepsilon}^p_{ij,k} \tag{12}$$

Based on the crystallographic analysis presented in the previous section, it is obvious from equations (7) and (9) that one should consider the effects of both $\nabla\boldsymbol{\varepsilon}^p$ and ∇p in the development of scale-dependent plasticity such that one cannot exist without the other. Hence, the author believes that for a complete constitutive description at small length scales, the internal power and the Helmholtz free energy should not include only the effects of $\dot{\boldsymbol{\varepsilon}}^p$ and $\dot{p}$ but should also include the effects of $\nabla\dot{\boldsymbol{\varepsilon}}^p$ and $\nabla\dot{p}$. Although these variables may 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 macro scale). For example dislocation interactions are observed on a mesolevel with length scale $0.1–10\mu m$ affecting strongly the material behaviour on the macro level with length scale $\geq 100\mu m$. 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.

3.1 Principle of virtual power

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 **n** denotes the outward unit normal to $\partial\Gamma$. The external expenditure of power is assumed to arise from a macroscopic surface traction **t**, the micro traction stress tensor, **m**, conjugate to $\dot{\boldsymbol{\varepsilon}}^p$, defined for each unit vector **n** normal on the boundary $\partial\Gamma$ of Γ. One, therefore, can write the external virtual power in the following form:

$$P_{\text{ext}} = \int_{\partial\Gamma} \left(t_i \delta v_i + m_{ij} \delta \dot{\varepsilon}^p_{ij} \right) \mathrm{d}A \tag{13}$$

The kinematical fields $\delta\mathbf{v}$, $\delta\dot{\boldsymbol{\varepsilon}}^p$ and $\delta\dot{p}$ are considered here as virtual, where δ is the variation parameter and **v** is the velocity vector.

The external power is balanced by an internal expenditure of power characterised by the Cauchy stress tensor $\boldsymbol{\sigma}$ defined over Γ for all time, the backstress **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 incorporates the gradients of the plastic strain, one also considers power expenditures associated with kinematic variables $\nabla\boldsymbol{\varepsilon}^p$ and ∇p. One, therefore, can assume that additional power is expended internally by the higher-order micro stress **S** conjugate to $\nabla\boldsymbol{\varepsilon}^p$ and the higher-order micro force vector **Q**

conjugate to ∇p. Specifically, the internal virtual power is assumed to have the following form:

$$P_{\text{int}} = \int_{\Gamma} \left(\sigma_{ij} \delta \dot{\varepsilon}_{ij}^{e} + X_{ij} \delta \dot{\varepsilon}_{ij}^{p} + R \delta \dot{p} + S_{ijk} \delta \dot{\varepsilon}_{ij,k}^{p} + Q_k \delta \dot{p}_{,k} \right) \mathrm{d}V \tag{14}$$

and to balance P_{ext}, equation (13), in the sense that $P_{\text{ext}} = P_{\text{int}}$.

Substituting equations $(11)_3$, (12), (13), and (14) along with $\dot{\boldsymbol{\varepsilon}}^{e} = \dot{\boldsymbol{\varepsilon}} - \dot{\boldsymbol{\varepsilon}}^{p}$ into the virtual power balance, $P_{\text{ext}} = P_{\text{int}}$, and then applying the divergence theorem yields, after some lengthy manipulations, the following result:

$$\begin{aligned} &\int_{\Gamma} \sigma_{ij,j} \delta v_i \, \mathrm{d}V + \int_{\partial\Gamma} \left(t_i - \sigma_{ij} n_j \right) \delta v_i \, \mathrm{d}A + \int_{\Gamma} \left[\tau_{ij} - X_{ij} + S_{ijk,k} - \left(R - Q_{k,k} \right) N_{ij} \right] \delta \dot{\varepsilon}_{ij}^{p} \, \mathrm{d}V \\ &+ \int_{\partial\Gamma} \left[m_{ij} - \left(S_{ijk} + Q_k N_{ij} \right) n_k \right] \delta \dot{\varepsilon}_{ij}^{p} \, \mathrm{d}A = 0 \end{aligned} \tag{15}$$

where $\boldsymbol{\tau}$ is the deviatoric part of $\boldsymbol{\sigma}$ (i.e., $\tau_{ij} = \sigma_{ij} - \sigma_{\text{kk}} \delta_{ij}/3$).

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

$$\sigma_{ij,j} = 0, \quad t_i = \sigma_{ij} n_j \tag{16}$$

$$\tau_{ij} - X_{ij} + S_{ijk,k} - \left(R - Q_{k,k} \right) N_{ij} = 0, \quad m_{ij} = \left(S_{ijk} + Q_k N_{ij} \right) n_k \tag{17}$$

According to the notion of Gurtin (2003), equation $(16)_1$ expresses the *macro force balance*, equation $(16)_2$ defines the stress vector as the surface density of the forces imposes which also provides the local *macro traction boundary conditions* on forces, equation $(17)_1$ is the *micro force balance* detailed in the next subsection, and equation $(17)_2$ is the *micro traction condition*, which is a higher-order internal boundary condition augmented by the interaction of dislocations across interfaces. The micro traction condition, equation $(17)_2$, is the soul of this paper as presented in Subsection 3.3.

3.2 Non-local plasticity yield surface

One can view the *micro force balance* in equation $(17)_1$ as the plasticity non-local yield condition. By taking the Euclidean norm $\| \ \|$ of equation $(17)_1$, the non-local plasticity loading surface f can then be expressed as:

$$f = \left\| \tau_{ij} - X_{ij} + S_{ijk,k} \right\| - R + Q_{k,k} = 0 \tag{18}$$

where $\mathbf{N}$ is collinear with $\boldsymbol{\tau} - \mathbf{X} + \text{div}\ \mathbf{S}$, $\| R - Q_{k,k} \| = R - Q_{k,k}$, and $\|\mathbf{N}\| = 1$. It is obvious that equation (18) represents a sphere in deviatoric stress-space of radius $R - \text{div}\ \mathbf{Q}$ centred at $\mathbf{X} - \text{div}\ \mathbf{S}$. One can also notice that the higher-order stress div $\mathbf{S}$ is a backstress quantity giving rise to additional kinematic hardening, while the micro stress div $\mathbf{Q}$ is giving rise to additional isotropic hardening (i.e., strengthening).

3.3 Interfacial effects

It will be shown here that the microscopic boundary condition in equation $(17)_1$ is related to the interfacial energy at free surfaces (e.g., the surface of a freestanding thin film, the

free surface of a void) or interfaces (e.g., the film-substrate interface, grain boundaries, inclusion interface).

Interfacial energy in small-scale systems (e.g., thin films, nano wires) is significant and cannot be ignored when the surface-to-volume ratio becomes large enough. For submicron and nano length scales the surface-to-volume ratio is appreciable. In equation $(17)_2$, the micro traction stress $\mathbf{m}$ is meant to be the driving force at the material internal and external boundaries, which can be interpreted as the *interfacial stress* at free surface or interface which is conjugate to the surface plastic strain. Therefore, $\mathbf{m}$ can be related to the interfacial energy φ per unit surface area by using the well-known relation (see Gurtin and Murdoch, 1978):

$$m_{ij} = \frac{\partial \varphi\left(\boldsymbol{\varepsilon}^{p}\right)}{\partial \varepsilon_{ij}^{p(S)}} \text{ on } \partial\Gamma^{p} \tag{19}$$

where $\boldsymbol{\varepsilon}^{p(S)}$ is the surface plastic strain and $\partial\Gamma^{p}$ is the plastic surface. Continuity of the strain field requires $\boldsymbol{\varepsilon}^{p}\big|_{\partial\Gamma^{p}} = \boldsymbol{\varepsilon}^{p(S)}$ at the interface. The components of $\boldsymbol{\varepsilon}^{p(S)}$ 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. $\varphi = 0$ designates a free surface where dislocations are allowed to escape, while $\varphi \to \infty$ designates a micro-clamped surface (i.e., rigid interface) where dislocations are not allowed to go through.

Hence, constrained plastic flow could be modeled either as a full constraint, i.e., $\boldsymbol{\varepsilon}^{p} = 0$ (when $\varphi \to \infty$), or no constraint, i.e., $\mathbf{m} = 0$ (when $\varphi \to 0$). However, following the ideas presented by Gudmundson (2004), Aifantis and Willis (2005), and Abu Al-Rub et al. (2007), an intermediate kind of micro-boundary condition is introduced. Therefore, the surface energy φ presented in equation (19) can be assumed to have the following quadratic form:

$$\varphi = \tfrac{1}{2} h \ell_S \varepsilon_{ij}^{p(S)} \varepsilon_{ij}^{p(S)} \text{ on } \partial\Gamma^{p} \tag{20}$$

where ℓ_S is a microstructural length scale that is related to boundary layer thickness and characterises the stiffness of the interface boundary in resisting plastic deformation. If $\ell_S = 0$, the interface would behave like a free surface and one obtains a micro-free boundary condition (i.e., $\mathbf{m} = 0$). On the other hand, if $\ell_S \to \infty$ then it would represent a condition for fully constrained dislocation movement at the interface and one obtains a micro-clamped boundary condition (i.e., $\boldsymbol{\varepsilon}^{p} = 0$).

The micro traction stress at the boundary, $\mathbf{m}$, can then be obtained from equations (19) and (20) as:

$$m_{ij} = h \ell_S \varepsilon_{ij}^{p(S)} \text{ on } \partial\Gamma^{p} \tag{21}$$

The micro traction stress is thus collinear with the plastic strain at the interface.

3.4 Application of the non-local Clausius-Duhem inequality

A thermodynamic procedure similar to the one advanced by Abu Al-Rub et al. (2007) is briefly pursued here. Assuming isothermal conditions for simplicity, the non-local Clausius-Duhem inequality is cast in the form:

$$\sigma_{ij}\dot{\varepsilon}_{ij} - \rho\dot{\Psi} + \mathbb{R} \geq 0 \tag{22}$$

The term $\mathbb{R}$ designates the non-locality energy residual that results from long-range micro structural interactions between the material points in the active plastic zone and interfaces, such that:

$$\int_{\Gamma} \mathbb{R}\,\mathrm{d}V = \int_{\partial\Gamma} \dot{\varphi}\,\mathrm{d}A = \int_{\partial\Gamma} m_{ij}\dot{\varepsilon}^{p}_{ij}\,\mathrm{d}A \tag{23}$$

Substituting equation $(17)_2$ and then applying the divergence theorem gives $\mathbb{R}$ as:

$$\mathbb{R} = S_{ijk,k}\dot{\varepsilon}^{p}_{ij} + S_{ijk}\dot{\varepsilon}^{p}_{ij,k} + Q_{k,k}\dot{p} + Q_{k}\dot{p}_{,k} \tag{24}$$

which shows that in the absence of gradients, one retains the local Clausius-Duhem inequality such that $\mathbb{R} = 0$.

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

$$\Psi = \Psi^{e}\left(\varepsilon^{e}_{ij}\right) + \Psi^{p}\left(\varepsilon^{p}_{ij}, p, \varepsilon^{p}_{ij,k}, p_{,k}\right) \tag{25}$$

On expanding the time derivative of equation (25) and substituting the result into equation (22) along the use of equation (24), one obtains the following thermodynamic state laws:

$$\sigma_{ij} = \rho\frac{\partial\Psi^{e}}{\partial\varepsilon^{e}_{ij}},\;\; X_{ij} = \rho\frac{\partial\Psi^{p}}{\partial\varepsilon^{p}_{ij}},\;\; R = \sigma_{y} + \rho\frac{\partial\Psi^{p}}{\partial p},\;\; S_{ijk} = \rho\frac{\partial\Psi^{p}}{\partial\varepsilon^{p}_{ij,k}},\;\; Q_{k} = \rho\frac{\partial\Psi^{p}}{\partial p_{,k}} \tag{26}$$

where σ_y is the size-dependent initial yield strength.

In order to develop equations amenable to the analysis and computation, one now considers a simple example for the definition of the Helmholtz free energy function. Both Ψ^e and Ψ^p that appear in equation (25) can be assumed to have, respectively, the following analytical form:

$$\rho\Psi^{e} = \tfrac{1}{2}\varepsilon^{e}_{ij}E_{ijkl}\varepsilon^{e}_{kl},\;\; \rho\Psi^{p} = \frac{h}{m+2}\left(\frac{e}{\varepsilon_{y}}\right)^{m+2}\varepsilon_{y}{}^{2} + \tfrac{1}{2}a\left(\varepsilon^{p}_{ij}\varepsilon^{p}_{ij} + \ell^{2}\varepsilon^{p}_{ij,k}\varepsilon^{p}_{ij,k}\right) \tag{27}$$

where **E** is the symmetric fourth-order elastic stiffness tensor, h, $m > 0$, and a are material constants, and ε_y is the yield strain. The parameter e is the generalised total accumulation of plastic strain and plastic strain gradients that is intended to measure the total dislocation density (SSDs and GNDs) (see e.g., Fleck et al., 1994; Gurtin, 2003, Gudmundson, 2004; Abu Al-Rub and Voyiadjis, 2004), which is defined by:

$$e^{2} = p^{2} + \ell^{2}p_{,k}p_{,k} \tag{28}$$

where ℓ is the bulk material length scale parameter used for dimensional consistency. Abu Al-Rub and Voyiadjis (2004, 2006) and Voyiadjis and Abu Al-Rub (2005) have shown that this length scale is not fixed but depends on the mean free path of dislocation such that it evolves with the coarse of plastic deformation. However, in this work, this length scale is assumed to be constant for simplicity.

Making use of equation (27) into equation (26) the following laws are obtained:

$$\sigma_{ij} = E_{ijkl}\left(\varepsilon_{kl} - \varepsilon_{kl}^{p}\right), \;\; X_{ij} = a\varepsilon_{ij}^{p}, \;\; R = \sigma_y + h\left(\frac{e}{\varepsilon_y}\right)^{m} p \tag{29}$$

$$S_{ijk} = a\ell^2 \varepsilon_{ij,k}^{p}, \;\; Q_k = h\ell^2 \left(\frac{e}{\varepsilon_y}\right)^{m} p_{,k} \tag{30}$$

Substituting the above equations into the yield function f, equation (18), one can then write:

$$f = \left\| \tau_{ij} - a\varepsilon_{ij}^{p} + a\ell^2 \nabla^2 \varepsilon_{ij}^{p} \right\| - \sigma_y - h\left(\frac{e}{\varepsilon_y}\right)^{m} p + h\ell^2 \frac{\partial}{\partial x_k}\left[\left(\frac{e}{\varepsilon_y}\right)^{m} p_{,k}\right] = 0 \tag{31}$$

where ∇^2 designates the Laplacian operator. In the absence of plastic strain gradients, the classical von-Mises criterion is retrieved. Furthermore, by setting $a = m = 0$, one obtains the gradient plasticity yield function of Aifantis (1984).

It should be emphasised that the non-local yield function in equation (31) should be supplemented by the microscopic boundary condition expressed by equation (21).

4 Application to size effects in thin films

This section presents an application of the proposed gradient plasticity model to handle size effects in metallic thin films. This model is used to investigate the size-dependent behaviour in biaxial loading of a plastic thin film on an elastic substrate. However, since cyclic loading is not considered here, kinematic hardening introduced by the conjugate forces **X** and **S** are neglected.

A biaxially loaded isotropic elasto-plastic thin film of thickness t on a thick semi-infinite elastic substrate is considered as shown in Figure 1(a). 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_o such that $\varepsilon_{11} = \varepsilon_{22} = \varepsilon_o$. A plane stress situation is assumed such that the non-vanishing stress and plastic strain components are:

$$\sigma_{11} = \sigma_{22} = \sigma_o\left(x_3\right), \;\; \varepsilon_{11}^{p} = \varepsilon_{22}^{p} = -\tfrac{1}{2}\varepsilon_{33}^{p} = \varepsilon_o^{p}\left(x_3\right) \tag{32}$$

The effective plastic strain $p = \sqrt{\varepsilon_{ij}^{p}\varepsilon_{ij}^{p}}$ and its gradient $p_{,k}$ are given by:

$$p = \sqrt{6}\varepsilon_o^{p}, \;\; p_{,k} = \sqrt{6}\varepsilon_{o,3}^{p} \tag{33}$$

where $\varepsilon_{o,3}^{p} = \partial\varepsilon_o^{p}/\partial x_3$. The stress-strain relationship can be simply obtained from the generalised Hook's law, equation $(29)_1$, as:

$$\sigma_o\left(x_3\right) = \left[E/(1-\nu)\right]\left[\varepsilon_o - \varepsilon_o^{p}\left(x_3\right)\right] \tag{34}$$

For simplicity and in order to obtain a closed form solution for the plastic strain, the exponent m in equation (31) is set to zero. Then, substituting equations (32), (33), and (34) into the yield condition, equation (31), yields the following ordinary differential equation for $\varepsilon_o^p\left(x_3\right)$:

$$\varepsilon_{o,33}^p-\left[\frac{1}{\ell^2}+\frac{E}{3(1-\nu)h\ell^2}\right]\varepsilon_o^p=\frac{\sigma_y}{\sqrt{6}h\ell^2}-\frac{E}{3(1-\nu)h\ell^2}\varepsilon_o \tag{35}$$

where $\varepsilon_{o,33}^p=\partial^2\varepsilon_o^p\big/\partial x_3^2$. It is convenient to express the above equation in a non-dimensional form with the aid of variable substitution (i.e., $z=x_3/t$, $\overline{\varepsilon}_o^p=\varepsilon_o^p\big/\varepsilon_y$, and $\overline{\varepsilon}_o=\varepsilon_o\big/\varepsilon_y$ with $\varepsilon_y=\sigma_y(1-\nu)\big/E$ being the in-plane yield strain) such that:

$$\overline{\varepsilon}_{o,zz}^p-\lambda^2\overline{\varepsilon}_o^p=-F \tag{36}$$

with constant coefficients λ and F are given by:

$$\lambda^2=\frac{1}{(\ell/t)}\sqrt{1+\frac{E}{3(1-\nu)h}},\quad F=\frac{E\left(\overline{\varepsilon}_o-\sqrt{3/2}\right)}{3(1-\nu)h(\ell/t)^2} \tag{37}$$

The interfacial energy effect as described by equation (21) is used now to prescribe the micro-boundary conditions at the film free surface and interface. The micro traction stress **m** can be obtained from equations $(17)_2$ and $(29)_5$ as:

$$m_{11}=m_{22}=-\tfrac{1}{2}m_{33}=h\ell^2\varepsilon_{o,3}^p \tag{38}$$

It is assumed that the micro traction stress **m** vanishes at the free surface ($x_3 = t$) such that equation (38) results in the following micro free boundary condition:

$$\frac{\partial\overline{\varepsilon}_o^p}{\partial z}=0 \text{ at } z=1 \tag{39}$$

The boundary condition at the film-substrate interface is given from equations (21) and (38) as follows:

$$(\ell_S/\ell)\overline{\varepsilon}_o^p=(\ell/t)\frac{\partial\overline{\varepsilon}_o^p}{\partial z} \text{ at } z=0 \tag{40}$$

Solving the ordinary differential equation, equation (36), which is subjected to the boundary conditions in equations (39) and (40), one obtains a closed-form expression for $\overline{\varepsilon}_o^p\left(z\right)$ as:

$$\overline{\varepsilon}_o^p\left(z\right)=\frac{F}{\lambda^2}\left[1-\frac{\cosh\lambda(1-z)}{\cosh\lambda+\delta\sinh\lambda}\right] \tag{41}$$

where $\delta=\lambda(\ell/t)(\ell/\ell_S)$.

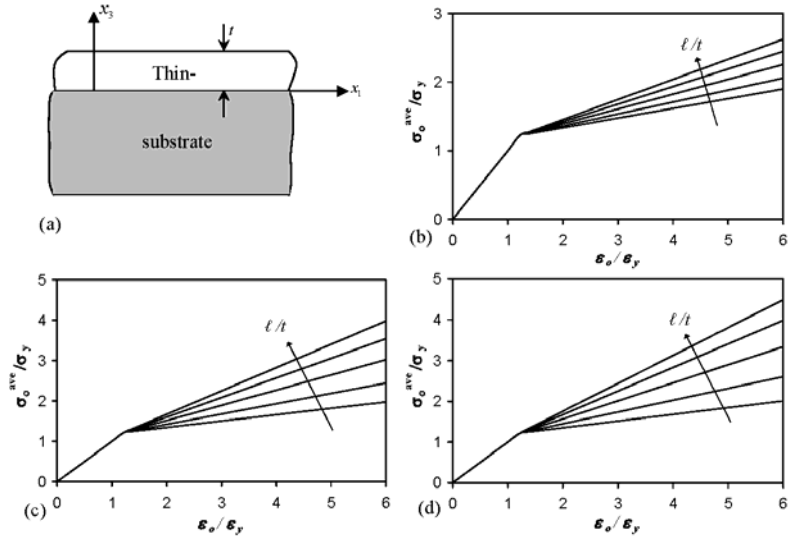
Substituting equation (41) back into the normalised expression of equation (34) (i.e., thein-plane stresses are normalised by the yield stress σ_y such that $\overline{\sigma}_o=\overline{\varepsilon}_o-\overline{\varepsilon}_o^p$), and then integrating the result for z from zero to one, one finds the following expression for the average stress in the film, $\overline{\sigma}_o^{\text{ave}}$, as:

$$\bar{\sigma}_o^{\text{ave}} = \bar{\varepsilon}_o - \frac{E\left(\bar{\varepsilon}_o - \sqrt{3/2}\right)}{3(1-\nu)h + E}\left[1 - \frac{\tanh\lambda}{\lambda\left(1+\delta\tanh\lambda\right)}\right]\mathrm{H}\left(\bar{\varepsilon}_o - \sqrt{3/2}\right) \tag{42}$$

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

Results in Figures 1 and 2 are presented for $h(1 - \nu)/E = 0.05$ and $\nu = 0.3$. Different film thickness are represented by ℓ / 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 $\ell_S/\ell = 1$, 10, and ∞ corresponding to soft, intermediate, and hard interfaces, respectively.

Figure 1 (a) Biaxial tension of a thin-film on a substrate. The average biaxial stress vs. biaxial strain for: (b) soft interface ($\ell_S/\ell = 1$), (c) intermediate interface $\ell_S/\ell = 10$, and (d) hard interface ($\ell_S/\ell \to \infty$)



Note: Different film thickness are represented by ℓ / t =0.1, 0.5, 1, 1.5, 2.

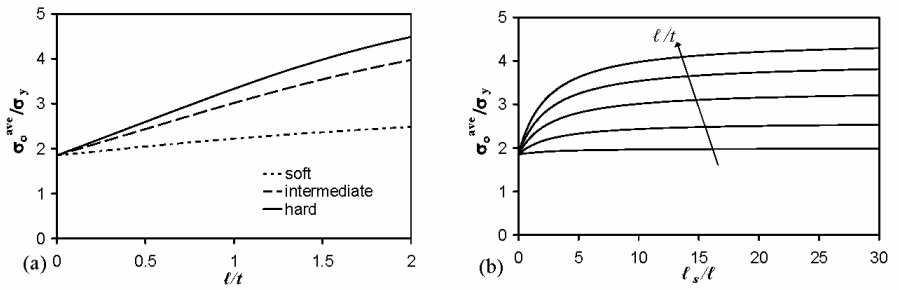
In Figures 1(b)–(d), normalised results for average film stress, equation (42), versus applied biaxial strain ε_o are presented. It is clearly seen that the hardening tangent modulus and the film stress increase with decreasing the film thickness, which agree qualitatively with the experimental observations. 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. Actually the results in Figure 1(d) coincide with the results for a rigid interface, i.e. no plastic strain at the interface. Similar trends have been obtained by Fredriksson and Gudmundson (2005).

The observed behaviour can be attributed to the less plastic deformation that is allowed at the interface as the interfacial energy increases (i.e., for higher ℓ_S/ℓ). In other words, as the interfacial 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 Figure 2(a) show that the hard interface reveals a pronounced size effect as compared to the soft and intermediate interfaces.

Figure 2(b) shows that $\ell_S / \ell = 0$ corresponds to the classical solution such that the interface behaves like a free surface (i.e., no size effect), whereas for $\ell_S / \ell \to \infty$ corresponds to a rigid interface and a pronounced size effect is observed. Furthermore, for a fixed film thickness, it can be noted from Figure 2(b) that the interfacial energy effect is significant when ℓ_S is in the order of ℓ such that for $\ell_S \gg \ell$ that interface behaves like a rigid surface where dislocation are completely blocked.

Figure 2 Average biaxial stress at a strain of $\varepsilon_o = 6\varepsilon_y$ vs. (a) normalised film thickness, (b) normalised interface stiffness



It can be noted if one plots the plastic strain distribution, equation (41), across the film thickness that 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.

5 Conclusions

In this paper, 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 is developed based on some dislocation mechanics interpretations. It is argued that the gradient of the plastic strain tensor, $\varepsilon^p_{ij,k}$, 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 GNDs. The thermodynamic conjugate force associated with $\varepsilon^p_{ij,k}$ 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. It is shown that interfacial effects can be considered by relating the micro tractions at interfaces to the interfacial energy which is dependent on the plastic strain at the interface. This is an important aspect for further development of gradient-dependent plasticity that is capable of modelling size effects in micro/nano-systems that are initially subjected to uniform

strains. It is shown that the existence of both gradients and interfacial energies contribute to the observed size effects.

It is concluded from the biaxial tension of the film-substrate system, in which the material is initially homogenous, that in the absence of the interfacial energy, 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. Therefore, if continuum theories are to be used to predict plastic behaviour at the micron or submicron length scales, a higher-order theory with interfacial energies is likely to be required.

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