50th AIAA/ASME/ASCE/AHS/ASC Structures, Structural Dynamics, and Materials Conference
17th
4 - 7 May 2009, Palm Springs, California

AIAA 2009-2593

Interfacial Plasticity Governs Strength Size-Scale Effects in Micro/Nanostructured Metals

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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 affect 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 [1, 2] for a complete list of references).

Therefore, it is well-known by now through intensive experimental studies that have been performed at the micron and nano length scales that the material mechanical properties strongly depend on the size of specimen and the microstructural features. The classical continuum mechanics fails to address this problem since no material length scale exists in its constitutive description. On the other hand, nonlocal continuum theories of integral-type or gradient-type have been to a good extent successful in predicting this type of size effect. However, they fail to predict size effects when strain gradients are minimal such as in the Hall-Petch effect. This problem is the main focus of this work. The effect of the material microstructural interfaces increase 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 higher-order gradient-dependent plasticity theory that enforces microscopic boundary conditions at interfaces and free surfaces. These nonstandard boundary conditions relate the microtraction stress at the interface to the interfacial energy. Application of the proposed framework to size effects in shear loading of a thin-film on an elastic substrate is presented. Three film-interface conditions are modeled: soft, intermediate, and hard interfaces.

I. Higher-Order Gradient Plasticity Theory

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 now to account for the effect of plastic strain gradients on the homogenized 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. The theory of Abu Al-Rub et al. [3] is recalled here.

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Based on the crystallographic dislocation basis presented by Abu Al-Rub et al. [3] it is shown that both the gradients of the plastic strain tensor, $\nabla\boldsymbol{\varepsilon}^{p}$, and the effective plastic strain, ∇p, should enter the definition of the internal virtual power besides their corresponding local parts; i.e. $\boldsymbol{\varepsilon}^{p}$ and p, such that one cannot exist without the other. Therefore, the principle of virtual power, which 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), can be expressed as follows:

$$\int_{\Gamma}\left(\sigma_{ij}\delta\dot{\varepsilon}_{ij}^{e}+X_{ij}\delta\dot{\varepsilon}_{ij}^{p}+R\delta\dot{p}+S_{ijk}\delta\dot{\varepsilon}_{ij,k}^{p}+Q_{k}\delta\dot{p}_{,k}\right)\mathrm{d}V=\int_{\partial\Gamma}\left(t_{i}\delta v_{i}+m_{ij}\delta\dot{\varepsilon}_{ij}^{p}\right)\mathrm{d}A \tag{1}$$

where $\boldsymbol{\sigma}$ is the Cauchy stress, $\boldsymbol{\varepsilon}^{e}=\boldsymbol{\varepsilon}-\boldsymbol{\varepsilon}^{p}$ is the elastic strain with $\boldsymbol{\varepsilon}$ being the total strain and $\boldsymbol{\varepsilon}^{p}$ is the plastic strain, $\mathbf{X}$ is the backstress associated with local kinematic hardening, R is the drag-stress associated with local isotropic hardening, $\mathbf{S}$ is a higher-order stress associated with nonlocal kinematic hardening, $\mathbf{Q}$ is a higher-order force associated with nonlocal isotropic hardening, $\mathbf{t}$ is the macroscopic surface traction, $\mathbf{v}$ is the velocity vector, $\mathbf{m}$ is a higher-order moment stress that is prescribed at the surface boundary $\partial\Gamma$ with an outward unit normal $\mathbf{n}$. Note that δ is the variation parameter used here to designate a virtual quantity, the superimposed dot designates the derivative with respect to time, and the comma is used to designate a derivative with respect to x_{k}.

Substituting $\dot{\boldsymbol{\varepsilon}}^{e}=\dot{\boldsymbol{\varepsilon}}-\dot{\boldsymbol{\varepsilon}}^{p}$, $\dot{\boldsymbol{\varepsilon}}=\nabla\otimes\mathbf{v}$, and $\dot{\boldsymbol{\varepsilon}}^{p}=\dot{p}\mathbf{N}$, with $\mathbf{N}$ being the direction of the plastic strain (i.e. the plasticity flow rule) where its magnitude is $\|\mathbf{N}\|=1$, into the virtual power balance, Eq. (1), and then applying the divergence theorem yields, after some lengthy manipulations, the following results:

$$\begin{aligned}&\int_{\Gamma}\sigma_{ij,j}\delta v_{i}\,\mathrm{d}V+\int_{\partial\Gamma}\left(t_{i}-\sigma_{ij}n_{j}\right)\delta v_{i}\,\mathrm{d}A+\int_{\Gamma}\left[\tau_{ij}-X_{ij}+S_{ijk,k}-\left(R-Q_{k,k}\right)N_{ij}\right]\delta\dot{\varepsilon}_{ij}^{p}\,\mathrm{d}V\\&+\int_{\partial\Gamma}\left[m_{ij}-\left(S_{ijk}+Q_{k}N_{ij}\right)n_{k}\right]\delta\dot{\varepsilon}_{ij}^{p}\,\mathrm{d}A=0\end{aligned} \tag{2}$$

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

$$\sigma_{ij,j}=0,\quad t_{i}=\sigma_{ij}n_{j} \tag{3}$$

$$\tau_{ij}-X_{ij}+S_{ijk,k}-\left(R-Q_{k,k}\right)N_{ij}=0,\qquad m_{ij}=\left(S_{ijk}+Q_{k}N_{ij}\right)n_{k} \tag{4}$$

where $\boldsymbol{\tau}$ is the deviatoric part of $\boldsymbol{\sigma}$. According to the notion of Gurtin [4], Eq. $(3)_1$ expresses the *macroforce balance*, Eq. $(3)_2$ defines the stress vector as the surface density of the forces imposes which also provides the local *macrotraction boundary conditions* on forces, Eq. $(4)_1$ is the *microforce balance*, and Eq. $(4)_2$ is the *microtraction condition*, which is a higher-order internal boundary condition augmented by the interaction of dislocations across interfaces. The microtraction condition, Eq. $(4)_2$, is the soul of this paper as is shown next.

By taking the Euclidian norm of Eq. $(4)_1$ one can show that the microforce balance is the nonlocal form of the von-Mises plasticity yield function such that:

$$\left\|\tau_{ij}-X_{ij}+S_{ijk,k}\right\|-R+Q_{k,k}=0 \tag{5}$$

The constitutive equations for the thermodynamic forces $\boldsymbol{\sigma}$, $\mathbf{X}$, $\mathbf{S}$, R, and $\mathbf{Q}$ can be obtained by making use of the nonlocal Clausius-Duhem inequality [3, 5]:

$$\sigma_{ij}\dot{\varepsilon}_{ij} - \rho\dot{\Psi} + \mathbb{R} \geq 0 \tag{6}$$

where $\Psi = \Psi(\boldsymbol{\varepsilon}^e, \boldsymbol{\varepsilon}^p, p, \nabla\boldsymbol{\varepsilon}^p, \nabla p)$ is the Helmholtz free energy which is a function of the local and nonlocal internal variables, ρ is the material density, and $\mathbb{R}$ designates the nonlocality energy residual that results from nonlocal long-range microstructural interactions between the material points in the active plastic zone and interfaces given by

$$\mathbb{R} = \left(S_{ijk}\dot{\varepsilon}^p_{ij} + Q_k\dot{p}\right)_{,k} \tag{7}$$

which shows that in the absence of gradients, one retains the local Clausius-Duhem inequality such that $\mathbb{R} = 0$. Substituting the time derivative of Ψ into Eq. (6) along with Eq. (7) yields:

$$\sigma_{ij} = \rho\frac{\partial\Psi}{\partial\varepsilon^e_{ij}},\quad X_{ij} = \rho\frac{\partial\Psi}{\partial\varepsilon^p_{ij}},\quad R = \sigma_y + \rho\frac{\partial\Psi}{\partial p}\ ,\quad S_{ijk} = \rho\frac{\partial\Psi}{\partial\varepsilon^p_{ij,k}},\quad Q_k = \rho\frac{\partial\Psi}{\partial p_{,k}} \tag{8}$$

where σ_y is the size-dependent initial yield strength. If one assumes the following quadratic form for Ψ:

$$\rho\Psi = \tfrac{1}{2}\varepsilon^e_{ij}E_{ijkl}\varepsilon^e_{kl} + \tfrac{1}{2}h\varepsilon^p_{ij}\varepsilon^p_{ij} + \tfrac{1}{2}hp^2 + \tfrac{1}{2}h\ell^2\varepsilon^p_{ij,k}\varepsilon^p_{ij,k} + \tfrac{1}{2}h\ell^2 p_{,k}p_{,k} \tag{9}$$

where $\mathbf{E}$ is the symmetric fourth-order elastic stiffness tensor, h is the plasticity hardening modulus, and ℓ is the material length scale, then one can express the nonlocal yield condition in Eq. (5) as follows:

$$f = \left\|\tau_{ij} - h\varepsilon^p_{ij} + h\ell^2\nabla^2\varepsilon^p_{ij}\right\| - \sigma_y - hp + h\ell^2\nabla^2 p = 0 \tag{10}$$

where ∇^2 designates the Laplacian operator. In the absence of plastic strain gradients, the classical von-Mises criterion is retrieved.

II. Interfacial Energy Effect

Interfacial energy in small-scale systems (e.g. thin films, nano wires, nanocomposites) is significant and cannot be ignored when the surface-to-volume ratio becomes large enough. In Eq. $(4)_2$, the microtraction 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 [3, 6, 7]:

$$m_{ij} = \partial\varphi(\boldsymbol{\varepsilon}^p)\big/\partial\varepsilon^{p(I)}_{ij} \quad \text{on } \partial\Gamma^p \tag{11}$$

where $\boldsymbol{\varepsilon}^{p(I)}$ is the interfacial plastic strain and $\partial\Gamma^p$ is the plastic interface. $\varphi = 0$ 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 $\varphi \to \infty$). The surface energy φ presented in Eq. (11) can be assumed to have the following form:

$$\varphi = \tfrac{1}{2}\ell_I\left(\sigma_y\left\|\varepsilon^{p(I)}_{ij}\right\| + h\varepsilon^{p(I)}_{ij}\varepsilon^{p(I)}_{ij}\right) \quad \text{on } \partial\Gamma^p \tag{12}$$

where σ_y is the bulk (size-independent) yield strength, h is the strain hardening modulus, and ℓ_I is a interfacial length scale that is related to the boundary layer thickness and characterizes the stiffness of the interface boundary in resisting plastic deformation. If $\ell_I = 0$, 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 $\ell_I \to \infty$ 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 microtraction stress at the boundary, $\mathbf{m}$, can then be obtained from Eqs. (11) and (12) as

$$m_{ij} = \ell_I \left(\sigma_y \varepsilon_{ij}^{p(I)} \big/ \| \varepsilon_{mn}^{p(I)} \| + h \varepsilon_{ij}^{p(I)} \right) \text{ on } \partial\Gamma^p \tag{13}$$

where if $\varepsilon_{ij}^{p(I)} = 0$, then $m_{ij} = \pm \ell_I \sigma_y \delta_{ij}$ such that $\ell_I \sigma_y$ characterizes the interfacial yield strength. Therefore, Eq. (13) physically characterizes a bulk-like yield condition at the interface, which governs the plasticity at the interface.

III. Application to Uniaxial loading of a thin film on a substrate

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 behavior in uniaxial loading of a plastic thin film on an elastic substrate [see Figure 1(a)]. The nonlocal yield function in Eq. (10) is solved numerically using the finite element algorithm for gradient plasticity as detailed in Abu Al-Rub and Voyiadjis [8]. Readers are referred to this paper for more details.

Results in Figs. 1(b) and 1(c), 2(a), and 2(b) are presented for h/E =0.2 for film thicknesses, where E is the Young's modulus, as represented by ℓ / d =0.1, 0.5, 1, 1.5, and 2. The level of interfacial energy at the interface is controlled by the normalized ratio ℓ_I / ℓ. Figs. 1(b) and 1(c) show the non-uniform plastic strain distribution across the film thickness d and the average stress-strain relation for $\ell_I / \ell = 1.0$. It is obvious from Figure 1(c) that both the overall yield strength of the film and the strain hardening rate increase with decreasing the characteristic size d. This response conforms qualitatively to the experimentally observed stress-strain response at the micron and submicron length scales [9]. In further results which are not reported here, a maximum increase in the yield strength and the strain hardening rate is obtained by assuming a rigid interface where dislocations are not allowed to transmit across the interface but instead piles-up there. Softer responses are obtained by reducing the interfacial strength. This indicates that for a rigid interface, d alone (represented by the ratio ℓ / d) controls the increase in the yield strength, whereas for compliant and intermediate interfaces both d and ℓ_I determine the yield strength and strain hardening rate.

Finally, one concludes that 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 microtractions 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 modeling size effects in micro/nano-systems. It is shown that the existence of both gradients and interfacial energies contribute to the observed size effects.

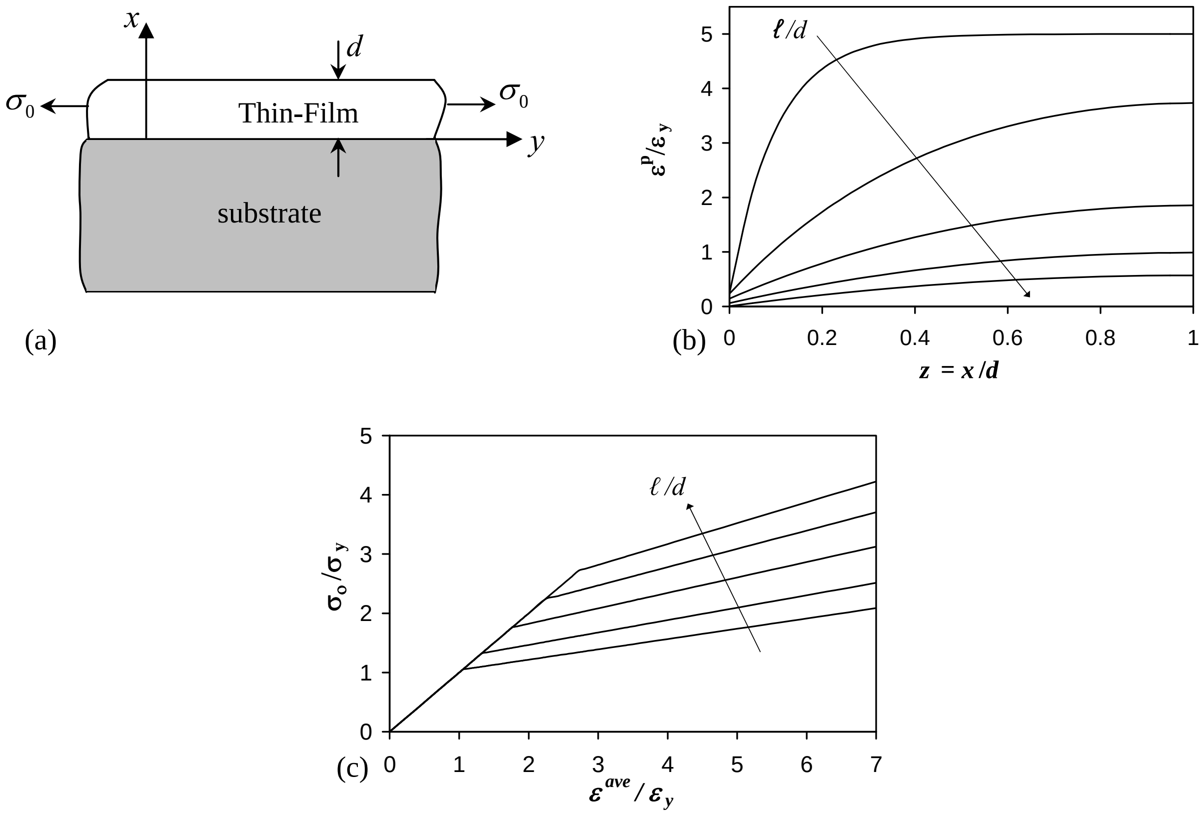

Fig. 1. (a) thin-film on an elastic substrate subjected to uniaxial tension. (b) Normalized plastic strain distribution along d for $\sigma_0/\sigma_y = 2$ and $\ell_I/\ell = 1.0$. (C) Normalized stress-strain relations for $\ell_I/\ell = 1.0$. Different sizes are represented by ℓ/d =0.1, 0.5, 1, 1.5, 2.

IV. Acknowledgements

The authors acknowledge the financial support by the US National Science Foundation under grant number CMMI-0728032.

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