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The finite deformation theory of Taylor-based nonlocal plasticity

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Abstract

Recent experiments have shown that metallic materials display significant size effect at the micron and sub-micron scales. This has motivated the development of strain gradient plasticity theories, which usually involve extra boundary conditions and possibly higher-order governing equations. We propose a finite deformation theory of nonlocal plasticity based on the Taylor dislocation model. The theory falls into Rice's theoretical framework of internal variables [J Mech Phys Solids 19 (1971) 433], and it does not require any extra boundary conditions. We apply the theory to study the micro-indentation hardness experiments, and it agrees very well with the experimental data over a wide range of indentation depth. © 2003 Elsevier Ltd. All rights reserved.

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1. Introduction

Recent experiments have repeatedly shown that metallic materials display significant size effect at the micron and submicron scales such as the micro-indentation hardness experiments (Nix, 1989, 1997; Guzman et al., 1993; Stelmashenko et al., 1993; Atkinson, 1995; Ma and Clarke, 1995; Poole et al., 1996; McElhaney et al., 1998; Suresh et al., 1999; Saha et al., 2001; Tymiak et al., 2001; Swadener et al., 2002; Lou et al., 2003), micro-twist (Fleck et al., 1994) and micro-bend experiments (Stolken and Evans, 1998; Haque and Saif, 2003; Shrotriya et al., 2003), particle-reinforced

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metal-matrix composite materials (Lloyd, 1994), and metallic materials containing microvoids (Taylor et al., 2002). Discrete dislocation simulations have also shown strong size dependence of material behavior at the micron scale (Cleveringa et al., 1997, 1998, 1999a, b; Shu et al., 2001). Classical theories of plasticity have no intrinsic material lengths, and cannot explain the observed size dependence of materials. This has motivated the development of strain gradient plasticity theories (e.g., Fleck and Hutchinson, 1993, 1997; Fleck et al., 1994; Gao et al., 1999a,b; Acharya and Bassani, 2000; Acharya and Beaudoin, 2000; Chen and Wang, 2000, 2002; Gurtin, 2000, 2002, 2003; Huang et al., 2000a,b; Beaudoin and Acharya, 2001; Jiang et al., 2001; Qiu et al., 2001, 2003; Evers et al., 2002; Hwang et al., 2002, 2003; Mariano, 2002; Dai and Parks, 2003; Wang et al., 2003). Alternatively, Gao and Huang (2001) developed a nonlocal plasticity theory based on the Taylor dislocation model (Taylor, 1934, 1938). The intrinsic material length established from the dislocation model is $(\mu/\sigma_{\rm Y})^2 b$, which is on the order of microns, where μ is the shear modulus, $\sigma_{\rm Y}$ is the yield stress, and b is the Burgers vector. This Taylor-based nonlocal theory of plasticity (TNT) does not require extra boundary conditions since the equilibrium equations are identical to those in classical plasticity (Gao and Huang, 2001). TNT plasticity has been shown to agree well with the aforementioned micro-scale experiments (Gao and Huang, 2001; Guo et al., 2001). Recently, Bazant and Guo (2002) investigated the asymptotic limit of TNT plasticity at the small scale. Tvergaard and Niordson (2003) developed a nonlocal plasticity theory to study the void size effect.

In this paper we develop a finite deformation theory for TNT plasticity since the effect of finite deformation is important not only in the aforementioned micro-scale experiments but also in material instability (e.g., plastic flow localization) and crack tip field. The proposed theory falls into the theoretical framework of internal variables established by Rice (1971), and it is applied to study the micro-indentation hardness experiments.

2. Finite deformation constitutive law of TNT plasticity

For a rate-independent material at constant temperature, Green strain **E** is a function of the second Piola–Kirchhoff stress **T**, $\mathbf{E} = \mathbf{E}$ (**T**, ξ), where ξ is an internal variable (or collection of internal variables) characterizing the state of internal rearrangement (Rice, 1971). The increment of **E** is decomposed to the elastic and plastic parts,

$$\dot{\mathbf{E}} = \dot{\mathbf{E}}^{e} + \dot{\mathbf{E}}^{p} = \mathbf{M} : \dot{\mathbf{T}} + \dot{\mathbf{E}}^{p}, \tag{1}$$

where $\mathbf{M} = \left(\frac{\partial \mathbf{E}}{\partial \mathbf{T}}\right)_{\xi}$ is the fourth-order tensor of elastic compliances; $\dot{\mathbf{E}}^{p} = \left(\frac{\partial \mathbf{E}}{\partial \xi}\right)_{\mathbf{T}}\dot{\xi}$ is the plastic strain rate which results solely from the change of internal variable (i.e., internal rearrangement). Since the Green strain \mathbf{E} can be generally expressed in terms of the Gibbs free energy Ψ_{G} (per unit volume in the reference configuration) as $\mathbf{E} = -\frac{\partial \Psi_{G}(\mathbf{T},\xi)}{\partial \mathbf{T}}$, the plastic strain rate can be written as

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$$\dot{\mathbf{E}}^{\mathrm{p}} = -\frac{\partial^{2}\Psi_{\mathrm{G}}(\mathbf{T},\xi)}{\partial\mathbf{T}\partial\xi}\dot{\xi} = \frac{\partial f}{\partial\mathbf{T}}\dot{\xi},\tag{2}$$

where $f = -\frac{\partial \Psi_G(\mathbf{T},\xi)}{\partial \xi}$ is the thermodynamic force associated with the internal variable. Eq. (2) is the same as the normality of plastic flow in classical plasticity if the thermodynamic force f associated with the internal variable is taken as the yield function. An example of f is the Von Mises effective stress τ_{eq} ,

$$f = \tau_{\rm eq}.$$
 (3)

In the present study, we take τ_{eq} as the effective stress in the current configuration, $\tau_{eq} = \left(\frac{3}{2}\boldsymbol{\tau}':\boldsymbol{\tau}'\right)^{1/2}$, where $\tau'_{ij} = \tau_{ij} - \frac{1}{3}\tau_{kk}\delta_{ij}$ is the deviatoric part of the Kirchhoff stress τ_{ij} . Since $\boldsymbol{\tau}$ is related to the second Piola–Kirchhoff stress \mathbf{T} via the deformation gradient \mathbf{F} by $\boldsymbol{\tau} = \mathbf{F} \cdot \mathbf{T} \cdot \mathbf{F}^{\mathsf{T}}$, the effective stress can be expressed in terms of \mathbf{T} by

$$\tau_{\rm eq} = \left[\frac{3}{2} \operatorname{tr} (\mathbf{C} \cdot \mathbf{T}^* \cdot \mathbf{C} \cdot \mathbf{T}^*)\right]^{1/2}.$$
(4)

where tr is the first invariant of the second order tensor, C = I + 2E is the right Cauchy–Green strain tensor, I is the identity tensor, and

$$\mathbf{T}^* = \mathbf{T} - \frac{1}{3} (\mathbf{T} : \mathbf{C}) \mathbf{C}^{-1}$$
(5)

The tensor $\frac{\partial f}{\partial \mathbf{T}}$ in (2) can then be obtained, $\frac{\partial f}{\partial \mathbf{T}} = \frac{\partial \tau_{eq}}{\partial \mathbf{T}} \mathbf{C} \cdot \mathbf{T}^* \cdot \mathbf{C}$, which gives the plastic strain rate in the reference configuration from (2) as

$$\dot{\mathbf{E}}^{p} = \frac{3}{2\tau_{eq}} \mathbf{C} \cdot \mathbf{T}^{*} \cdot \mathbf{C} \dot{\boldsymbol{\xi}}.$$
(6)

The physical meaning of the internal variable ξ now becomes clear. The push forward of (6) gives the plastic strain rate in the current configuration, $\mathbf{d}^{\mathrm{p}} = \mathbf{F}^{-T} \cdot \dot{\mathbf{E}}^{\mathrm{p}} \cdot \mathbf{F}^{-1} = \frac{3\pi'}{2\tau_{\mathrm{eq}}} \dot{\xi}$. The equivalent plastic strain rate is then obtained,

$$\dot{\boldsymbol{\epsilon}}^{\mathrm{p}} = \left(\frac{2}{3}\mathbf{d}^{\mathrm{p}}:\mathbf{d}^{\mathrm{p}}\right)^{1/2} = \dot{\boldsymbol{\xi}},\tag{7}$$

which indicates that the internal variable ξ is the (accumulative) equivalent plastic strain $\xi = \epsilon^{p} = \int \dot{\epsilon}^{p} dt$.

The yield function in TNT plasticity is (Gao and Huang, 2001)

$$\tau_{\rm eq} = \sigma(\epsilon^{\rm p}, \eta), \tag{8}$$

where τ_{eq} is the effective stress in the current configuration, and is given in (4) for finite deformation; σ is the flow stress given by (Huang et al., 2000b; Gao and Huang, 2001)

$$\sigma = \sigma_{\rm ref} \sqrt{f_p^2(\epsilon^{\rm p}) + l\eta}.$$
(9)

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Here $\sigma = \sigma_{\text{ref}} f_p(\epsilon^p)$ is the stress-plastic strain relation in uniaxial tension, σ_{ref} is a reference stress (e.g., yield stress), η is the effective strain gradient to be given later, l is the intrinsic material length given in terms of the shear modulus μ and Burgers vector b by

$$l = 18\alpha^2 \left(\frac{\mu}{\sigma_{\rm ref}}\right)^2 b,\tag{10}$$

and α is an empirical material constant around 0.3 in the Taylor dislocation model (Taylor, 1934, 1938). It should be pointed out that, even though the intrinsic material length *l* depends on the reference stress σ_{ref} , the flow stress (and TNT plasticity) does not since (9) can be rewritten as $\sigma = \sqrt{\left[\sigma_{ref}f_p(\epsilon^p)\right]^2 + 18\alpha^2\mu^2 b\eta}$.

The effective strain gradient η in (9) is determined from the dislocation models as $\eta^2 = \frac{1}{4}\eta'_{ijk}\eta'_{ijk}$ (Gao et al., 1999b; Gao and Huang, 2001), where $\eta'_{ijk} = \eta_{ijk} - \frac{1}{4}(\delta_{ik}\eta_{jpp} + \delta_{jk}\eta_{ipp})$ is the deviatoric strain gradient tensor; the strain gradient tensor η_{ijk} is obtained by integrating its rate, $\eta_{ijk} = \int \dot{\eta}_{ijk} dt$; $\dot{\eta}_{ijk}$ is defined in terms of the corresponding Jaumann rate η in order to ensure the objectivity of η

$$\dot{\eta}_{ijk} = \stackrel{\nabla}{\eta}_{ijk} + w_{ip}\eta_{pjk} + w_{jp}\eta_{ipk} + w_{kp}\eta_{ijp},\tag{11}$$

and the Jaumann rate is given by

$$\stackrel{\vee}{\eta}_{ijk} = d_{jk,i} + d_{ik,j} - d_{ij,k}.$$
 (12)

Here **w** and **d** are the anti-symmetric and symmetric parts of the velocity gradient in the current configuration, respectively, $d_{ij} = \frac{1}{2} \left(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i} \right)$. In the nonlocal theory of plasiticity, $d_{ij,k}$ is evaluated via the nonlocal integral of **d** (Gao and Huang, 2001)

$$d_{ij,k}(\mathbf{x}) = \int_{V_{\text{cell}}} \left[d_{ij}(\mathbf{x} + \zeta) - d_{ij}(\mathbf{x}) \right] \zeta_m \mathrm{d}V \left[\int_{V_{\text{cell}}} \zeta_m \zeta_k \mathrm{d}V \right]^{-1}, \tag{13}$$

where x is a material point in the current configuration, V_{cell} is the integration cell surrounding x, and ζ is the local coordinate origined at x. The increment of the effective strain gradient can be obtained as

$$\dot{\eta} = \frac{1}{4\eta} \eta'_{ijk} \eta'_{ijk} = \frac{1}{4\eta} \eta'_{ijk} {\stackrel{\nabla}{\eta}}_{ijk}.$$
(14)

The yield function can be rewritten from (4), (8) and (9) as

$$f_{\text{yielding}} \equiv \frac{3}{2} \operatorname{tr}(\mathbf{C} \cdot \mathbf{T}^* \cdot \mathbf{C} \cdot \mathbf{T}^*) - \sigma_{\text{ref}}^2 \Big[f_p^2(\epsilon^p) + l\eta \Big] = 0.$$
(15)

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Its increment form gives the consistency condition to determine the equivalent plastic strain rate $\dot{\epsilon}^{p}$ since $\dot{\eta}$ is known from (14).

The substitution of (6), (7) and the consistency condition from (15) into (1) gives the rate of Green strain $\dot{\mathbf{E}}$ in terms of the rate of second Piola–Kirchhoff stress $\dot{\mathbf{T}}$. Its inverse gives the constitutive law of finite deformation TNT plasticity,

$$\dot{\mathbf{T}} = \mathbf{L} : \left\{ \dot{\mathbf{E}} - \alpha' \frac{\mathbf{C} \cdot \mathbf{T}^* \cdot \mathbf{C} \ f_{\text{loading}}}{\frac{4}{9} \sigma_{\text{ref}}^2 f_p(\epsilon^p) f'_p(\epsilon^p) \sigma + (\mathbf{C} \cdot \mathbf{T}^* \cdot \mathbf{C}) : \mathbf{L} : (\mathbf{C} \cdot \mathbf{T}^* \cdot \mathbf{C}) \right\},\tag{16}$$

where $L = M^{-1}$ is the fourth-order tensor of elastic moduli, and α' is the loading coefficient given by

$$\begin{aligned} \alpha' &= 1 & f_{\text{yielding}} = 0 \text{ and } f_{\text{loading}} > 0 \\ &= 0 & f_{\text{yielding}} < 0 \text{ or } f_{\text{loading}} < 0; \end{aligned} \tag{17}$$

 f_{yielding} is defined in (15), and

$$f_{\text{loading}} \equiv \left[(\mathbf{C} \cdot \mathbf{T}^* \cdot \mathbf{C}) : \mathbf{L} + \frac{2}{3} (\mathbf{T} : \mathbf{C}) \mathbf{T}^* + 2(\mathbf{T}^* \cdot \mathbf{C} \cdot \mathbf{T}^*) \right] : \dot{\mathbf{E}} - \frac{1}{3} \sigma_{\text{ref}}^2 l \dot{\eta}, \qquad (18)$$

which separates plastic loading from elastic unloading.

It should be pointed out that the equilibrium equations and boundary conditions in the finite deformation TNT plasticity are the same as their counterparts in the classical theory of plasticity, and are therefore not presented here.

3. Micro-indentation hardness experiments

Based on the principle of virtual work, we have implemented the finite deformation theory of TNT plasticity in the ABAQUS finite element program via its USER-ELEMENT subroutine UEL. Details of finite element implementation are very similar to those of Guo et al. (2001), who studied the micro-indentation hardness experiments via the infinitesimal deformation theory of TNT plasticity. We then use the finite element method for finite deformation theory of TNT plasticity to examine the effect of finite deformation in micro-indentation experiments.

Fig. 1 shows a schematic diagram of Guo et al.'s (2001) indentation model for McElhaney et al.'s (1998) micro-indentation hardness experiment of polycrystalline copper. The same indentation model is adopted in the present study, but the finite deformation theory of TNT plasticity is used. The indentation hardness H is defined as the average contact pressure P/A, where P is the indentation load and A is the contact area.

Fig. 2 shows the micro-indentation hardness predicted by the present study for polycrystalline copper. The square of the indentation hardness, $\left(\frac{H}{H_0}\right)^2$, is plotted against the inverse of indentation depth, $\frac{1}{h}$, as suggested by Nix and Gao (1998), where *H* is the micro-indentation hardness and H_0 is the indentation hardness for large depth of indentation (i.e., without strain gradient effects). The shear modulus

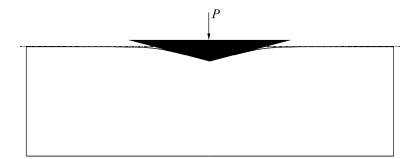


Fig. 1. A schematic diagram of the indentation model.

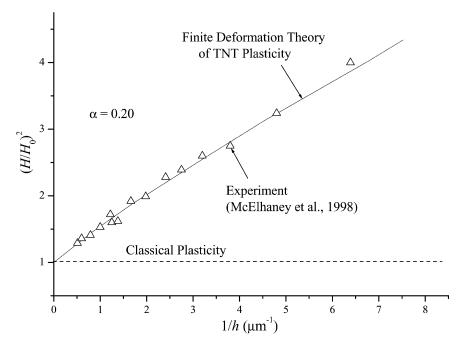


Fig. 2. Depth dependence of the hardness for polycrystalline copper. The solid line is the predicted hardness based on the finite deformation theory of TNT plasticity; *H* is the micro-indentation hardness, *h* is the depth of indentation, and $H_0 = 834$ MPa is the indentation hardness for a large indentation depth. The triangles are experimental data of McElhaney et al. (1998). Other material properties are shear modulus $\mu = 42$ GPa, Poisson's ratio $\nu = 0.3$, Burgers vector b = 0.255 nm, uniaxial stress–strain relation $\sigma = 518\epsilon^{0.3}$ MPa, and Taylor coefficient $\alpha = 0.20$.

of copper is $\mu = 42$ GPa, Poisson ratio $\nu = 0.3$ (McElhaney et al., 1998), Burgers vector b = 0.255 nm, and Taylor coefficient $\alpha = 0.2$. The uniaxial stress-strain relation after plastic yielding can be written as a power law, $\sigma = 518\epsilon^{0.3}$ MPa, where the work hardening exponent 0.3 is consistent with that reported by McLean (1962) and Fleck et al. (1994) for polycrystalline copper. Based on this uniaxial stress-strain relation, the finite element method predicts an indentation hardness $H_0 = 834$

MPa at a large indentation depth (without strain gradient effects), which agrees with the measured value of H_0 (McElhaney et al., 1998). The experimental hardness data of McElhaney et al. (1998) are also shown in Fig. 2 for comparison. It is clearly observed that the numerically predicted hardness based on the finite deformation theory of TNT plasticity agrees very well with the experimental data over a wide range of indentation depth, from one tenth of a micron to several microns. The Taylor coefficient $\alpha = 0.20$ in Fig. 1 for the finite deformation theory of TNT plasticity is smaller than its counterpart $\alpha = 0.30$ used by Guo et al. (2001) in the infinitesimal deformation heory of TNT plasticity. Therefore, finite deformation has some effect in micro-indentation experiments, and should be accounted for.

4. Concluding remarks

We have developed a finite deformation theory of nonlocal plasticity from the Taylor dislocation model. The theory falls into Rice's (1971) theoretical framework of internal variables, and it has the same equilibrium equations and therefore does not require additional boundary conditions. We have also applied the theory to study the micro-indentation hardness experiments, and established that the effect of finite deformation is important in the micro-indentation hardness experiments and should be accounted for.

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