DETERMINATION OF THE MATERIAL INTRINSIC LENGTH SCALE OF GRADIENT PLASTICITY THEORY

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Abstract: The enhanced strain-gradient plasticity theories formulate a constitutive framework on the continuum level that is used to bridge the gap between the micromechanical plasticity and the classical continuum plasticity. To assess the size effects it is indispensable to incorporate an intrinsic material length parameter into the constitutive equations. However, the full utility of gradient-type theories hinges on one's ability to determine the constitutive length-scale parameter. The classical continuum plasticity is unable to predict properly the evolution of the material flow stress since the local deformation gradients at a given material point are not accounted for. The gradient-based flow stress is commonly assumed to rely on a mixed type of dislocations: statistically stored dislocations (SSDs) and geometrically necessary dislocations (GNDs). In this work a micromechanical model to assess the coupling between SSDs and GNDs, which is based on the Taylor's hardening law, is used to identify the deformation-gradient-related intrinsic length-scale parameter in terms of measurable microstructural physical parameters. This work also presents a method for identifying the length-scale parameter from micro-indentation tests.

Key words: Gradient plasticity; Size effects; Intrinsic material length-scale; Geometrically necessary dislocations; Micro-hardness.

1. INTRODUCTION

In the last ten years a number of authors have physically argued that the size dependence of the material mechanical properties results from an

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increase in strain gradients inherent in small localized zones leads to geometrically necessary dislocations that cause additional hardening [1]. A number of gradient-enhanced theories have been proposed to address the size effects through incorporation of intrinsic length-scale measures in the constitutive equations, mostly based on continuum mechanics concepts [2,3].

Although there has been a tremendous theoretical work to understand the physical role of the gradient theory, this research area is still in a critical state with numerous controversies. This is due to some extent to the difficulty in calibration of the different material properties associated with the gradient-dependent models, which is impossible for certain cases. From dimensional consideration, in gradient-type plasticity theories, length scales are introduced through the coefficients of spatial gradients of one or more internal variables. Thus, the full utility of gradient-based models hinges on one's ability to determine the constitutive length parameter that scales the gradient effects. The work we report here aims at remedying this situation.

However, it is believed that the calibration of the constitutive coefficients of a gradient-dependent model should not only be based on stress-strain behavior obtained from macroscopic mechanical tests, but should also draw information from micromechanical gradient-dominant tests, such as micro-indentation and nano-indentation tests [4]. Nix and Gao [5] estimated the material length scale parameter ℓ from the micro-indentation experiments of McElhaney et al. [6] to be $\ell = 12\mu m$ for annealed single crystal copper and $\ell = 5.84\mu m$ for cold worked polycrystalline copper. By fitting micro-indentation hardness data, Begley and Hutchinson [7] have estimated that the material length-scale associated with the stretch gradients ranges from 0.25 to $0.5\mu m$, while the material lengths associated with rotation gradients are on the order of $4\mu m$.

Recently, Voyiadjis and Abu Al-Rub [8] developed a general thermodynamic framework for the analysis of heterogeneous media. They showed that the variety of plasticity and damage phenomena at small-scale level dictate the necessity of more than one length parameter in the gradient description. They expressed these material length-scales in terms of macroscopic measurable material parameters. However, this work concerns with the identification of the material intrinsic length-scale parameter ℓ for gradient isotropic hardening plasticity. This can be effectively done through establishing a bridge between the plasticity at the micromechanical scale with the plasticity at the macromechanical scale. This bridge is characterized by the gradient plasticity theories. This constitutive framework yields expressions for the deformation-gradient-related intrinsic length-scale parameter in terms of measurable microstructural physical parameters. Moreover, we present a method for identifying the material intrinsic length parameter from micro- and nano-indentation tests using conical or pyramidal indenters.

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2. BRIDGING OF LENGTH SCALES

Many researchers tend to write the non-local weak form of the conventional effective plastic strain, $\hat{p}$, in terms of its local counterpart, p, and high-order gradient terms. The following modular generalization of $\hat{p}$ can then be defined [2] by:

$$\hat{p} = \left[p^{\gamma} + (\ell\eta)^{\gamma} \right]^{1/\gamma} \tag{1}$$

where ℓ is a length parameter that is required for dimensional consistency and whose physical interpretation will be discussed in detail later in this paper. η is the measure of the effective plastic strain gradient of any order. The superimposed hat denotes the spatial non-local operator. γ is a constant which can be interpreted as a material parameter.

The critical shear stress that is required to untangle the interactive dislocations and to induce a significant plastic deformation is defined as the Taylor flow stress:

$$\tau = \left[\tau_S^{\beta} + \tau_G^{\beta} \right]^{1/\beta} \tag{2}$$

with τ_S and τ_G are given by the Taylor's hardening laws related to the SSD density, ρ_S, and GND density, ρ_G, respectively, as follows:

$$\tau_S = \alpha_S G b_S \sqrt{\rho_S} \tag{3}$$

$$\tau_G = \alpha_G G b_G \sqrt{\rho_G} \tag{4}$$

where b_S and b_G are the magnitudes of the Burgers vectors associated with SSDs and GNDs, respectively, G is the shear modulus, and α_S and α_G are statistical coefficients which account for the deviation from regular spatial arrangements of the SSD and GND populations, respectively. β is a constant which is interpreted as a material parameter similar to that of γ.

Expressing Eq. (2) in terms of Eqs. (3) and (4) yields a general expression for the overall flow stress in terms of an equivalent total dislocation density, ρ_T, such that:

$$\tau = \alpha_S G b_S \sqrt{\rho_T} \quad \text{with} \quad \rho_T = \left[\rho_S^{\beta/2} + \left(\alpha_G^2 b_G^2 \rho_G / \alpha_S^2 b_S^2 \right)^{\beta/2} \right]^{2/\beta} \tag{5}$$

Eq. (5) is expressed at the microscale; however, plasticity is the macroscopic outcome from the combination of many dislocation elementary properties at the micro and mesoscopic scales. One can then write the flow stress at the macroscopic scale using a power law ($\sigma = k\hat{p}^{1/m}$) and Eq. (1) as follows:

$$\sigma = k\left[p^{\gamma} + l^{\gamma}\eta^{\gamma} \right]^{1/m\gamma} \tag{6}$$

where γ, k, and m are material constants. It is important to emphasize that the non-local effects associated with the presence of local deformation gradients at a given material point are incorporated into Eq. (5) through the GNDs density, ρ_G, and Eq. (6) through the strain-gradient, η.

Generally, it is assumed that the total dislocation density, ρ_T, represents the total coupling between two types of dislocations which play a significant role in the hardening mechanism. Material deformation enhances dislocation formation, dislocation motion, and dislocation storage. Dislocation storage causes material hardening. Stored dislocations generated by trapping each other in a random way are referred to as statistically-stored dislocations (SSDs), while stored dislocations required for compatible deformation within the polycrystal 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 [3]. The SSDs are created by homogenous strain and are related to the plastic strain, while the GNDs are related to the curvature of the crystal lattice or to the strain gradients. Plastic strain gradients appear either because of geometry of loading or because of inhomogeneous deformation in the material. Hence, GNDs are required to account for the permanent shape change. The non-local effective plastic strain in Eq. (1) is intended to measure the total dislocation density that accounts for both: dislocations that are statistically stored and geometrically necessary dislocations induced by the strain gradients.

The gradient in the plastic strain field is accommodated by the GND density, ρ_G, so that the effective strain gradient η that appears in Eq. (1) can be defined as follows [3]:

$$\eta = \rho_G b_G / \bar{r} \tag{7}$$

where $\bar{r}$ is the Nye factor.

The plastic shear strain, γ^p, as a function of the SSD density, ρ_S, is defined as [9]:

$$\gamma^p = b_S L_S \rho_S \tag{8}$$

where L_S is the mean spacing between SSDs which is usually in the order of submicron. The plastic strain in the macroscopic plasticity theory is defined in terms of the plastic shear strain and an orientation tensor as follows [9]:

$$\varepsilon_{ij}^p = \gamma^p M_{ij} \tag{9}$$

where M_{ij} is the symmetric Schmidt's orientation tensor.

The flow stress σ is the conjugate of the effective plastic strain variable p in macro-plasticity. For proportional, monotonically increasing plasticity, p is defined as:

$$p = \sqrt{2\varepsilon_{ij}^p \varepsilon_{ij}^p / 3} \tag{10}$$

Hence, utilizing Eqs. (8) and (9) in Eq. (10) one can write p as a function of SSDs as follows:

$$p = b_S L_S \rho_S \bar{M} \tag{11}$$

where $\bar{M} = \sqrt{2M_{ij}M_{ij}/3}$ can b

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Substituting ρ_G and ρ_S from Eqs. (7) and (11), respectively, into $\sigma = \sqrt{3}\tau$, where τ is given by Eq. (5) yields the following expression for the flow stress:

$$\sigma = \alpha_S G\sqrt{3b_S/L_S\bar{M}}\left[p^{\beta/2} + \left(\alpha_G^2 b_G L_s \bar{M}\,\bar{r}/\alpha_S^2 b_S\right)^{\beta/2}\eta^{\beta/2}\right]^{1/\beta} \tag{12}$$

Comparing Eq. (12) with Eq. (6) yields the following relations:

$$\gamma = \mu,\quad m = 2,\quad k = \alpha_S G\sqrt{\frac{3b_S}{L_S\bar{M}}},\quad \ell = \left(\alpha_G/\alpha_S\right)^2\left(b_G/b_S\right)L_S\bar{M}\,\bar{r} \tag{13}$$

Substituting $L_S\bar{M}$ from Eq. $(13)_3$ into Eq. $(13)_4$ one can express the material intrinsic length parameter ℓ by:

$$\ell = 3\alpha_G^2 b_G \bar{r}\left(\frac{G}{k}\right)^2 \tag{14}$$

We note that the above equation implies that the length-scale parameter may vary with the strain-rate and temperature for a given material for the case $k = \hat{k}(\dot{p},T)$, where $\dot{p} = \sqrt{2\dot{\varepsilon}_{ij}^p\dot{\varepsilon}_{ij}^p/3}$. However, for most metals, the flow stress increases with the strain rate and decreases with temperature increase. Thus causing the intrinsic material length-scale to decrease with increasing strain-rates and to increase with temperature decrease. However, opposite behavior is concluded for the gradient term η.

3. IDENTIFICATION FROM MICRO-HARDNESS TESTS

It is well-known by now that indentation tests at scales on the order of one micron have shown that measured hardness increases significantly with decreasing indent size. This has been attributed to the evolution of GNDs associated with gradients. Consider the indentation by a rigid cone, as shown schematically in Figure 1. GND density can then be defined by [5]:

$$\rho_G = 3\tan^2\theta/2b_G h \tag{15}$$

where h is the indentation depth, and θ is the angle between the surface of the conical indenter and the plane of the surface. This angle is related to the indentation depth h and the radius of the contact area of the indentation a through the following relation, $\tan\theta = h/a$. Both h and a are measured in the unloaded configuration and characterized as the residual values after unloading.

The mapping from the hardness-indentation depth curve ($H-h$ curve, where H is the hardness) to the tensile stress-plastic strain curve ($\sigma-p$) is defined by [10]:

$$H=\kappa\sigma\,,\quad p=c(h/a)=c\tan\theta \tag{16}$$

where κ is the Tabor's factor of $\kappa=2.8$ [10] and c is a material constant on the order of $c=1$ [11].

The substitution of Eq. (5) into Eq. (16) with $\sigma=\sqrt{3}\tau$ and Eq. $(13)_4$ into Eq. (11), yield the following expressions for hardness, H, and the SSD density, ρ_S, respectively, as follows:

$$H=\sqrt{3}\,\kappa\alpha_S G b_S\left[\rho_S^{\beta/2}+\left(\alpha_G b_G/\alpha_S b_S\right)^{\beta}\rho_G^{\beta/2}\right]^{1/\beta} \tag{17}$$

$$\rho_S=c\bar{r}\alpha_G^2 b_G\tan\theta/\ell b_S^2\alpha_S^2 \tag{18}$$

Moreover, we can define the macro-hardness H_o as the hardness that would arise from SSDs alone in the absence of strain gradients, such that [5]:

$$H_o=\sqrt{3}\,\kappa\tau_S=\sqrt{3}\kappa\alpha_S G b_S\sqrt{\rho_S} \tag{19}$$

With these relations we can now write the micro-hardness for the conical/pyramidal indenter using Eqs. (16) - (19) as follows:

$$\left(H/H_o\right)^{\beta}=1+\left(h^*/h\right)^{\beta/2}\quad\text{with}\quad h^*=\zeta\ell\quad\text{and}\quad\zeta=3\tan^3\theta/2c\bar{r} \tag{20}$$

where h^* is a material specific parameter that characterizes the depth dependence of the hardness and depends on the indenter geometry as well as on the plastic flow. Eq. $(20)_2$ shows that h^* is a linear function of the length-scale parameter ℓ. Thus, h^* is a crucial parameter that characterizes the indentation size effects and its accurate experimental measure gives a reasonable value for the length-scale parameter ℓ obtained by using Eqs. $(20)_2$ and $(20)_3$. We note that if $\beta=2$ in Eq. (20), one retains the relation originally proposed in [5]. Moreover, substituting Eq. (18) into Eq. (19) along with Eq.(14), one can obtain a simple relation to predict the macro-hardness H_o as:

$$H_o=\kappa k\sqrt{c\tan\theta} \tag{21}$$

where k can be obtained from Eq. $(13)_3$.

The characteristic form for the depth dependence of the hardness presented by Eqs. (20) gives a straight line when the data are plotted as $(H/H_o)^{\beta}$ versus $h^{-\beta/2}$, the intercept of which is 1 and the slope is $h^{*\beta/2}$. The length-scale parameter $\ell=h^*/\zeta$ can then be calculated using Eq. $(20)_2$, where ζ is determined in terms of the shape of the conical indenter (i.e. $\tan\theta$) and the material properties (i.e. $\bar{r}$ and c) which are known. Therefore, by using Eq. (20) to fit the hardness experimental data obtained from indentation tests, one can simply compute the intrinsic length-scale parameter that characterizes the size effects.

Figure 1 shows that Eq. $(20)_1$ fits the hardness experimental data [4] very well for $\beta=2$. From the slope of the solid line, one obtains $h^*=1.538\mu m$

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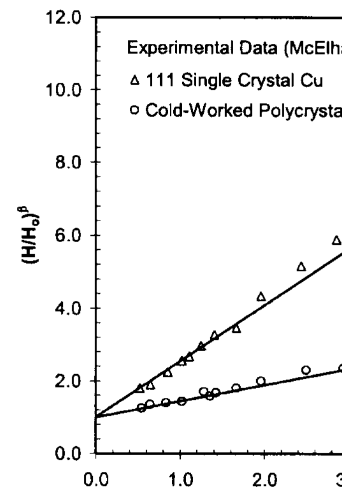

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for 111 single crystal annealed Cu and $h^* = 0.444\mu m$ for the cold-worked polycrystal Cu. Using Eqs. $(20)_2$ and $(20)_3$ for $\tan\theta = 0.358$, $\bar{r}=2$, $c=1$ we obtain $\zeta = 0.268$ and $\ell = 5.74\mu m$ for 111 single crystal annealed Cu and $\ell = 1.66\mu m$ for the cold-worked polycrystal Cu. A value of $\ell = 5.84\mu m$ has been reported in [5] for 111 single crystal annealed Cu and $\ell = 12\mu m$ for the cold-worked polycrystal Cu.

One can note that ℓ for the cold worked sample is smaller than the value for the annealed sample, indicating that spacing between statistically stored dislocations is reduced in the hardened-worked material. Apparently, numerical experiments of the indentation problem using finite element method are required to verify those findings.

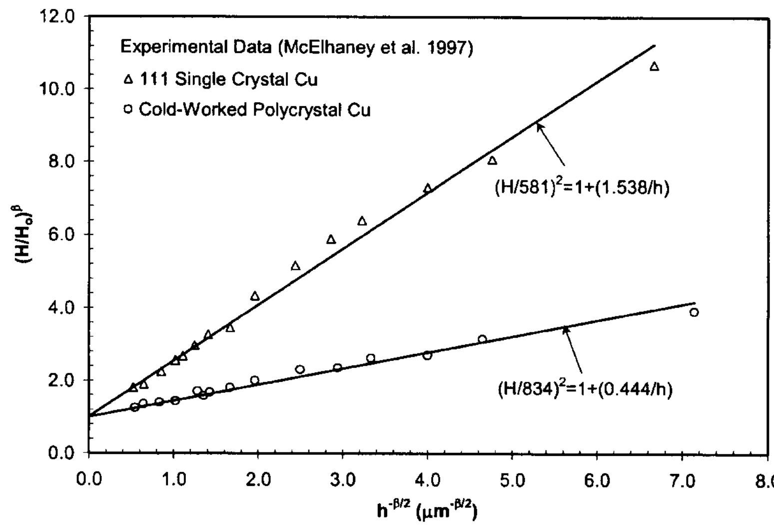

Figure 1. Comparison of the experimental results and the prediction of Eq. $(20)_1$ to determine the intrinsic material length scale for copper.

4. CONCLUSIONS

This work uses the gradient theory to bring the microstructural (described by the Taylor's hardening law) and continuum (described by the strain-hardening power law) descriptions of plasticity closer together in order to identify the material intrinsic length-scale parameter ℓ. As a result ℓ is defined in terms of the average distance between statistically stored dislocations L_S; the Nye factor $\bar{r}$; the Schmidt's orientation factor $\bar{M}$; the Burgers vector $\boldsymbol{b}$; and the empirical constant α.

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GRANULAR PACKIN

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Abstract Discrete element simulati
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1 INTRODUCTION

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