PERGAMON

Journal of the Mechanics and Physics of Solids
50 (2002) 435–448

JOURNAL OF THE
MECHANICS AND
PHYSICS OF SOLIDS

www.elsevier.com/locate/jmps

Scaling of dislocation-based strain-gradient plasticity

Zdeněk P. Bažant*

Departments of Civil Engineering and Materials Science, McCormick School of Engineering and Applied Science, Northwestern University, Evanston, IL 60208-3109, USA

Received 29 January 2001; received in revised form 3 May 2001; accepted 3 May 2001

Abstract

By taking into account the dislocations that are geometrically necessary for producing a curvature or twist of the atomic lattice in crystals, Gao et al. recently developed a theory of strain-gradient plasticity on the micrometer scale and showed that it agrees relatively well with the tests of hardness, torsion and bending of copper on the micrometer scale. This paper subjects this theory to an asymptotic scaling analysis. It is shown that the small-size asymptotic limit of this theory exhibits (1) an unusually strong size effect in which the corresponding nominal stresses in geometrically similar structures of different sizes D vary as $D^{-5/2}$, and (2) an asymptotic approach to a load-deflection diagram whose tangent stiffness gradually increases, starting with an infinitely small initial stiffness at infinitely small stress. Although this peculiar small-size asymptotic behavior might not be attainable within the practical applicability range of a continuum theory, it renders questionable any efforts to construct approximations of an asymptotic matching character, with a two-sided asymptotic support, which have previously been proven effective for quasibrittle materials such as concrete, rock, ice and fiber composites. A possible simple modification of the existing theory with respect to the small-size asymptotic properties is suggested. However, the questions of experimental justification of such a modification and its compatibility with the dislocation theory will require further study. The small-size asymptotic properties of other strain gradient theories of plasticity have not been analyzed, except for those of the previous Fleck-Hutchinson theory, which have been found reasonable.

Keywords: Metal plasticity; Strain gradient; Dislocations; Size effect; Scaling; Asymptotic methods; Micromechanics

* Corresponding author. Tel.: 847-491-4025; fax: +1-847-467-1078.
E-mail address: z-bazant@nwu.edu (Z.P. Bažant).

0022-5096/02/$ - see front matter
PII: S0022-5096(01)00082-5

1. Introduction

The recent interest in small-scale extensions of continuum models capturing the transition to atomic lattice models for metallic crystals and polycrystals brings about interesting problems of scaling. In these problems, one can exploit a formal analogy with the previous studies of scaling in quasibrittle heterogeneous materials such as concrete (e.g., Bažant and Planas 1998; Bažant and Chen 1997; Bažant 1997, 1999, 2001). Inspired by such analogy, this study will examine the scaling properties of the recent theory of Gao et al. (1999a), which is based on dislocations that are geometrically necessary for producing a curvature or twist of the atomic lattice.

2. Formulation of mechanism-based gradient plasticity

The strain gradient effects on elastic behavior were introduced in the phenomenological constitutive formulations of Toupin (1962) and Mindlin (1965), which extended the idea of Cosserat and Cosserat (1898). Departing from these early formulations, Fleck and Hutchinson (1993, 1997), Hutchinson (1997), Gao et al. (1999a, b) and Huang et al. (2000) presented an impressive series of progressively refined studies that culminated with a dislocation-based strain-gradient theory of metal plasticity. The theory that they developed was shown capable of reproducing the size effects observed in tests of micro-hardness, micro-torsion and micro-bending of copper on the scale of 0.2 to 200 μm.

The constitutive relation of strain gradient plasticity based on dislocations theory is given by Gao et al. (1999a, b) and Huang et al. (2000) in the following form:

$$\sigma_{ik} = K\delta_{ik}\varepsilon_{nn} + \frac{2\sigma}{3\varepsilon}\varepsilon'_{ik}, \tag{1}$$

$$\tau_{ijk} = l_\varepsilon^2\left(\frac{K}{6}\eta^H_{ijk} + \sigma\Phi_{ijk} + \frac{\sigma_Y^2}{\sigma}\Psi_{ijk}\right), \tag{2}$$

where

$$\Phi_{ijk} = \frac{1}{\varepsilon}(\Lambda_{ijk} - \Pi_{ijk}), \quad \Psi_{ijk} = f(\varepsilon)f'(\varepsilon)\Pi_{ijk}, \quad \varepsilon = \sqrt{\tfrac{2}{3}\varepsilon'_{ij}\varepsilon'_{ij}}, \quad \eta = \tfrac{1}{2}\sqrt{\eta_{ijk}\eta_{ijk}} \tag{3}$$

and

$$\Lambda_{ijk} = \tfrac{1}{72}[\eta_{ijk} + \eta_{kji} + \eta_{kij} - \tfrac{1}{4}(\delta_{ik}\eta_{ppj} + \delta_{jk}\eta_{ppi})], \tag{4}$$

$$\Pi_{ijk} = [\varepsilon_{ik}\eta_{jmn} + \varepsilon_{jk}\eta_{imn} - \tfrac{1}{4}(\delta_{ik}\varepsilon_{jp} + \delta_{jk}\varepsilon_{ip})\eta_{pmn}]\varepsilon_{mn}/54\varepsilon^2, \tag{5}$$

$$\eta^H_{ijk} = \tfrac{1}{4}(\delta_{ik}\eta_{jpp} + \delta_{jk}\eta_{ipp}). \tag{6}$$

Here K = elastic bulk modulus; $\varepsilon'_{ik} = \varepsilon_{ik} - \delta_{ik}\varepsilon_{nn}/3$ = deviatoric strains, $\varepsilon_{ik} = (u_{i,k} + u_{k,i})/2$ = strains; $\boldsymbol{\varepsilon}, \boldsymbol{\eta}$ = 2nd and 3rd order tensors of components $\varepsilon_{ij}, \eta_{ijk}$; $\eta_{ijk} = u_{k,ij} =$

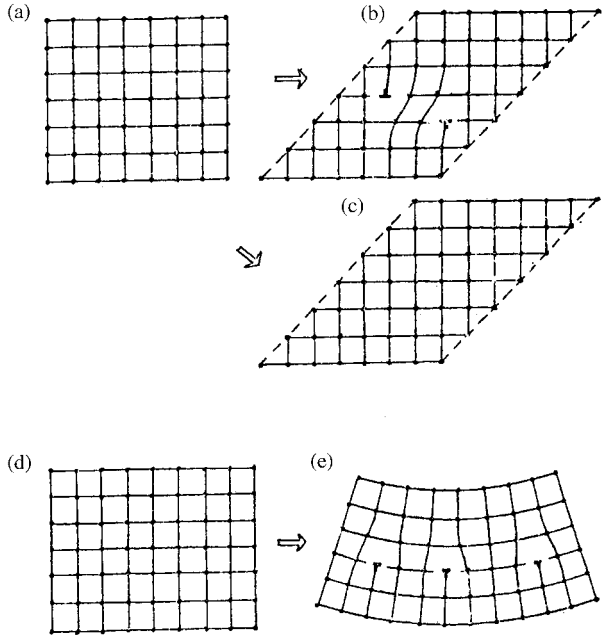

Fig. 1. Illustration of the difference between (b) statistically stored dislocations and (e) geometrically necessary dislocations; (a,d) show the initial states of square lattices with 56 and 63 atoms, respectively, and (c) shows that for a homogeneous deformation no dislocations are necessary.

displacement curvature (or twist), reflecting the effect of geometrically necessary dislocations (Fig. 1) [the strain gradient is $\varepsilon_{ij,k} = (\eta_{jki} + \eta_{ikj})/2$]; η^H_{ijk} = volumetric (hydrostatic) part of η_{ijk}; τ_{ijk} = third-order stresses work-conjugate to η_{ijk} (analogous to Cosserat's couple stresses, Cosserat and Cosserat, 1898). While Gao et al. (1999a, b) characterize the plastic constitutive properties by the semi-empirical formula

$$\sigma = \sigma_Y \sqrt{f^2(\varepsilon) + l\eta} \tag{7}$$

we will find it interesting to consider a slightly more general formula

$$\sigma = \sigma_Y [f^q(\varepsilon) + (l\eta)^p]^{1/q} \tag{8}$$

with positive exponents p and q (Gao et al.'s theory corresponds to the case $p = 1$, $q = 2$); σ_Y = yield stress, σ, ε = stress and strain intensities; η = effective strain gradient proportional to the density of geometrically stored dislocations (i.e., to lattice curvature or twist); $f(\varepsilon)$ = classical plastic hardening function, which reflects the effect of statistically stored dislocations and is an increasing function of a monotonically decreasing slope, $0 < f'(0) < \infty$; $l = \lambda_0 b$; $l_\varepsilon = \lambda_\varepsilon b$ = size of the so-called 'mesoscale cell' or the spacing of geometrically necessary dislocations (which is the material length characterizing the transition from standard to gradient plasticity and is interpreted by Gao et al. as the minimum volume on which the macroscopic deformation contributions of the geometrically necessary dislocations may be smoothed by a continuum); b = magnitude

of Burgers vector of edge or screw dislocation (e.g., 0.255 nm for copper); $\lambda_0, \lambda_\varepsilon =$ positive dimensionless material characteristics expressed in terms of Taylor factor, Nye factor and the ratio of elastic shear modulus to the dislocation reference stress (according to Gao et al.'s estimate, $\lambda_\varepsilon \approx 20,000$ for copper).

Assuming that not only the strains but also the strain gradients do work, one obtains from the principle of virtual work (or by minimization of Helmholtz free energy density) the following field equations of equilibrium (Gao et al., 1999a, b):

$$\sigma_{ik,i} - \tau_{ijk,ij} + f_k = 0. \tag{9}$$

3. Dimensionless variables

Let us now introduce the dimensionless variables (labeled by an overbar):

$$\bar{x}_i = x_i/D, \quad \bar{u}_i = u_i/D, \quad \bar{\varepsilon}_{ij} = \varepsilon_{ij}, \quad \bar{\eta}_{ijk} = \eta_{ijk}D, \quad \bar{\varepsilon} = \varepsilon, \quad \bar{\eta} = \eta D, \tag{10}$$

$$\bar{\sigma}_{ik} = \sigma_{ik}/\sigma_{\mathrm{Y}}, \quad \bar{\tau}_{ijk} = \tau_{ijk}/(\sigma_{\mathrm{Y}} l_\varepsilon), \quad \bar{\sigma} = \sigma/\sigma_{\mathrm{Y}}, \quad \bar{f}_k = f_k D/\sigma_{\mathrm{N}}. \tag{11}$$

While the derivatives with respect to x_i are denoted by subscript i preceded by a comma, the derivatives with respect to dimensionless coordinates will be denoted as $\partial_i = \partial/\partial\bar{x}_i$. By interchanging $\sigma_{\mathrm{Y}}, \sigma_{\mathrm{N}}$ and bulk modulus K, or D, l_ε and l, one could create many different sets of dimensionless variables. However, as will be seen, the choice of the set in Eqs. (10) and (11) happens to be the right one for determining the size effect.

To transform the field equations into dimensionless coordinates, we first note that, since η^H_{ijk}, Λ_{ijk} and Π_{ijk} are defined by Gao et al. (2000a, b) as homogeneous functions of degree 1 of tensors $\boldsymbol{\eta}$ and $\boldsymbol{\varepsilon}$, they transform as

$$\eta^H_{ijk} = \bar{\eta}^H_{ijk}/D, \quad \Lambda_{ijk} = \bar{\Lambda}_{ijk}/D, \quad \Pi_{ijk} = \bar{\Pi}_{ijk}/D \tag{12}$$

and so

$$\Phi_{ijk} = \bar{\Phi}_{ijk}/D, \quad \Psi_{ijk} = \bar{\Psi}_{ijk}/D. \tag{13}$$

$\bar{\Lambda}_{ijk}$, $\bar{\Pi}_{ijk}$, $\bar{\Phi}_{ijk}$, $\bar{\Psi}_{ijk}$ and $\bar{\eta}^H_{ijk}$ are given by the same expressions as (3), (4)–(6) except that all the arguments are replaced by the dimensionless ones, labeled by overbars.

We now substitute Eqs. (1) and (2) into Eq. (9) and thus, using Eqs. (10) and (11) and noting that $\partial/\partial x_i = (1/D)\partial_i$, we obtain the following dimensionless stresses and third-order stresses:

$$\bar{\sigma}_{ik} = \frac{K}{\sigma_{\mathrm{Y}}}\delta_{ik}\bar{\varepsilon}_{nn} + \frac{\bar{\sigma}}{\bar{\varepsilon}}\bar{\varepsilon}'_{ik}, \tag{14}$$

$$\bar{\tau}_{ijk} = \frac{\lambda_\varepsilon}{D}\left(\frac{K}{6\sigma_{\mathrm{Y}}}\bar{\eta}^H_{ijk} + \bar{\sigma}\bar{\Phi}_{ijk} + \frac{1}{\bar{\sigma}}\bar{\Psi}_{ijk}\right), \tag{15}$$

where

$$\bar{\sigma} = \left[f^q(\bar{\varepsilon}) + \left(\frac{l}{D}\bar{\eta}\right)^p\right]^{1/q}. \tag{16}$$

The field equations of equilibrium transform as

$$\partial_i \bar{\sigma}_{ik} - \frac{l_\varepsilon}{D} \partial_i \partial_j \bar{\tau}_{ijk} + \frac{\sigma_N}{\sigma_Y} \bar{f}_k = 0. \tag{17}$$

To avoid struggling with the formulation of the boundary conditions, consider first that they are homogeneous, i.e., the applied surface tractions and applied couple stresses vanish at all parts of the boundary where the displacements are not fixed as 0. All the loading characterized by nominal stress σ_N is applied as body forces f_k whose distributions are assumed to be geometrically similar; σ_N is considered as the parameter of these forces, varying proportionaly to σ_N. Then the transformed boundary conditions are also homogeneous. In terms of the dimensionless coordinates, the boundaries of geometrically similar structures of different sizes are identical.

4. Scaling and size effect

For $D/l_\varepsilon \to \infty$, which also implies $D/l \to \infty$, the dimensionless third-order stresses $\bar{\tau}_{ijk}$ vanish and all the equations reduce, as required, to the standard field equations of equilibrium on the macroscale.

Consider now the opposite asymptotic behavior for $D/l_\varepsilon \to 0$. We have

$$\bar{\sigma} \approx (\bar{\eta} \lambda_1 l_\varepsilon / D)^{p/q}. \tag{18}$$

After substituting Eqs. (14) and (15) into Eq. (17), we obtain the differential equations of equilibrium in the form:

$$\partial_i \left[\frac{K}{\sigma_Y} \delta_{ik} \bar{\varepsilon}_{nn} + \frac{1}{\bar{\varepsilon}} \left(\frac{l\bar{\eta}}{D} \right)^{p/q} \bar{\varepsilon}'_{ik} \right] - \left(\frac{l_\varepsilon}{D} \right)^2 \partial_i \partial_j \left[\frac{K}{6\sigma_Y} \bar{\eta}^H_{ijk} + \left(\frac{l\bar{\eta}}{D} \right)^{p/q} \bar{\Phi}_{ijk} + \left(\frac{D}{l\bar{\eta}} \right)^{p/q} \bar{\Psi}_{ijk} \right] = - \frac{\sigma_N}{\sigma_Y} \bar{f}_k. \tag{19}$$

Now we multiply this equation by $(D/l_\varepsilon)^{2+p/q}$ and take the limit of the left-hand side for $D \to 0$. This leads to the following asymptotic form of the field equations:

$$\partial_i \partial_j (\bar{\eta}^{p/q} \bar{\Phi}_{ijk}) = \chi \bar{f}_k, \quad \text{with } \chi = \lambda_1^{-p/q} \frac{\sigma_N}{\sigma_Y} \left(\frac{D}{l_\varepsilon} \right)^{2+p/q}, \tag{20}$$

where $\lambda_1 = \lambda_0/\lambda_\varepsilon$. Since D is absent from the foregoing field equation (and from the boundary conditions, too, because they are homogeneous), the dimensionless displacement field as well as parameter χ must be size independent. Thus, we obtain the following small-size asymptotic scaling law for the dislocation-based strain-gradient plasticity:

$$\sigma_N = \sigma_Y \chi \lambda_1^{p/q} \left(\frac{l_\varepsilon}{D} \right)^{2+p/q}, \tag{21}$$

where $\lambda_1 = \lambda_0/\lambda_\varepsilon =$ constant, and the exponent $2 + p/q > 2$. According to Gao et al.'s theory, $p/q = 1/2$, and so (Fig. 2 top)

$$\sigma_N \propto D^{-5/2}. \tag{22}$$

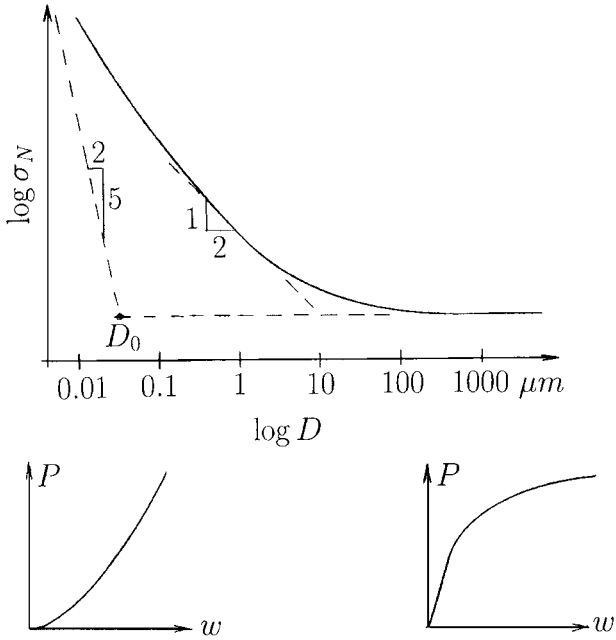

Fig. 2. (a) Size effect of the existing dislocation-based theory of strain gradient plasticity, and (b) strange load-deflection curve for the small-size limit implied by the existing dislocation-based theory of gradient plasticity for bodies deforming with a constant relative displacement profile.

As for the loading by applied surface tractions and applied couple stresses, one may consider them replaced by equivalent body forces f_k (proportional to σ_N) that act within a surface layer of a very small thickness δ proportional to D. In that case the preceding analysis applies. The limit process $\delta/D \to 0$ then proves in a simple way that (21) must also be valid for such loading.

The asymptotic size effect given by Eqs. (21) or (22) is curiously strong. It is much stronger than the size effect of linear elastic fracture mechanics (LEFM) for similar sharp cracks on the macroscale, which is $\sigma_N \propto D^{-1/2}$.

An interesting exception occurs for the case of pure bending. In that case, $\bar{\Phi}_{ijk}$ identically vanishes and the last dominant term in (19) shows that the asymptotic scaling law (22) must be replaced by $\sigma_N \alpha D^{-3/2}$. Such a size effect is still enviously strong.

5. Definition of comparable nominal stresses

When the structure is not at maximum load but is hardening, one must decide which are the σ_N values that are comparable and should be described by the scaling law (21). If the value of

$$(\sigma_N/\sigma_Y)(D/l_\varepsilon)^{2+p/q} \tag{23}$$

in the small-size asymptotic field Eq. (20) is given, then parameter χ is a constant, and (if the material model is physically realistic) the partial differential equation (20) with homogeneous boundary conditions must have one solution $\bar{u}_k$, with the corresponding $\bar{\varepsilon}_{ik}, \bar{\eta}_{kij}$. Hence, the dimensionless deformation field is the same for all sizes D. It follows that the σ_N values to which the scaling law (21) applies are those corresponding to the same norm of the relative (dimensionless) displacement, $||\bar{u}_k||$. The norm may for example be defined as the angle of twist of a cylinder, θ; or the maximum relative displacement $\bar{u}_{\max}$ in the body; or the maximum strain in the body; or the relative depth of indentation $\bar{h} = h/D$; or the relative displacement at any homologous points in the body.

The asymptotic field equation for $D/l_\varepsilon \to \infty$ is

$$\partial_i \bar{\sigma}_{ik} + \bar{f}_k \bar{\sigma}_N/\sigma_Y = 0 \tag{24}$$

in which

$$\bar{\sigma}_{ik} = (K/\sigma_Y)\delta_{ik}\bar{\varepsilon}_{nn} + (\bar{\sigma}/\bar{\varepsilon})\bar{\varepsilon}'_{ik}, \quad \bar{\sigma} = f(\bar{\varepsilon}). \tag{25}$$

Elimination of the stresses yields the field equation

$$\frac{K}{\sigma_Y}\delta_{ik}\partial_i\bar{\varepsilon}_{nn}\partial_i\left(\frac{f(\bar{\varepsilon})}{\bar{\varepsilon}}\bar{\varepsilon}'_{ik}\right) + \frac{\sigma_N}{\sigma_Y}\bar{f}_k = 0. \tag{26}$$

Now again, if the ratio σ_N/σ_Y is given, then (for a problem properly modeled physically) this partial differential equation with homogeneous boundary conditions must have one solution $\bar{\varepsilon}_{ik}$, corresponding to one field $\bar{u}_k$. It follows that the comparable σ_N values for different sizes are again those corresponding to the same norm of relative displacement, $||\bar{u}_k||$.

6. Small-size asymptotic load-deflection response

By virtue of the fact that the hardening function $f(\varepsilon)$ disappears from the field equation when it is reduced to its asymptotic form (20), it turns out that, for the theory of Gao et al. (1999), it is easy to determine the load-deflection curve for the special case in which the displacement distribution (or relative displacement profile) remains constant during the loading process. This is for example typical of the pure torsion test of a long circular fiber, in which, by arguments of symmetry, the tangential displacements must vary linearly along every radius.

For such loading, all the dimensionless displacements $\bar{u}_k$ at all the points in a structure of arbitrary but fixed geometry increase in proportion to a parameter w such that $\bar{u}_k = w\hat{u}_k$ where $\hat{u}_k$ is not only independent of D but also invariable during the proportional loading process. w may be considered as the displacement norm, $||\bar{u}_k||$.

Noting that η and Φ_{ijk} are homogeneous functions of degree 1 of both $\boldsymbol{\eta}$ and $\boldsymbol{\varepsilon}$, we may write for such deformation behavior

$$\bar{\eta} = w\hat{\eta}, \quad \bar{\Phi}_{ijk} = w\hat{\Phi}_{ijk}, \tag{27}$$

where $\hat{\eta}$ and $\hat{\Phi}_{ijk}$ are functions of dimensionless coordinates that do not change during the loading process at any small enough size D. Therefore, the asymptotic field Eq. (20)

may be rewritten as

$$\partial_i \partial_j \left(\hat{\eta}^{p/q} \hat{\Phi}_{ijk} \right) = \hat{f}_k, \quad \text{with } \hat{f}_k = \frac{f_k}{c_0} w^{-(1+p/q)}, \quad c_0 = \lambda_1^{p/q} \frac{\sigma_Y}{D} \left(\frac{l_\varepsilon}{D} \right)^{2+p/q}. \tag{28}$$

It follows from the field equation that if the relative displacement distribution (profile) $\hat{u}_k$ is constant during the loading process, as in pure bending of a slender beam or in torsion of a long cylinder, then the distribution $\hat{f}_k$ at the small-size limit must be constant as well. Using Eq. (28), we see that

$$f_k = c_0 \hat{f}_k w^{1+p/q}. \tag{29}$$

Since $c_0 \hat{f}_k$ is constant during loading, we must conclude that, for the small-size limit and for any loading with a constant relative displacement profile (as in pure bending or in torsion of a cylinder), the load-deflection curve is generally a power curve of exponent $1+(p/q) > 1$; for Gao et al.'s theory, the exponent is $\frac{3}{2}$ (Fig. 2 bottom left).

Now it is rather obvious that such a behavior is strange. The tangential stiffness of the structure for infinitely small stress is infinitely small, which is physically hard to accept, and then it increases with increasing deflection. An increase of tangential stiffness with increasing displacement (Fig. 2 bottom left) is of course seen in locking materials (such as rubber or cellular materials), but would be queer as a property attributed to metals, even at the small-size continuum limit.

Arbitrary positive exponents p and q were included in the definition of effective stress in order to check whether a change of p and q could remedy this problem. We see that the exponent of the power-law load-deflection curve can be made as close to 1 as desired but cannot be exactly 1. So a complete remedy cannot be achieved by this simple modification of Gao et al. (1999a, b) semi-empirical definition of stress intensity σ.

Thus, it seems that some more fundamental modification of Gao et al.'s (1999) theory might be desirable in order to eliminate the strangely strong asymptotic size effect.

In the interest of mathematical rigorosity, it may be noted that the asymptotic load-deflection curve (29) is not differentiable at the origin, $w=0$. In the case of two limits $D \to 0$ and $w \to 0$, one must pay attention to the physically correct sequence of taking these limits. The correct sequence is to fix an arbitrarily small D, then determine the load-deflection curve for that D, and finally examine what happens to the load-deflection curve as D approaches zero. In this regard, note that the five terms that are summed on the left-hand side of Eq. (19) are proportional, respectively, to the functions

$$w, \quad (w/D)^{p/q}, \quad w/D^2, \quad w^{1+p/q} D^{-p/q-2}, \quad w^{1-p/q} D^{p/q-2} \tag{30}$$

($0 < p/q < 1$ is assumed). Now, if D is very small but finite and if w approaches zero, then the dominant term will be the last one. So the load-deflection curve for very small D is of the type $w^{1-p/q}$, or $\sqrt{w}$ in Gao et al.'s theory, which means that the initial tangent is vertical and the initial stiffness infinite. However, for $D \to 0$, the load-deflection curve must approach formula (19) for which the initial tangent is horizontal, i.e., the initial stiffness is zero. This means that although the asymptotic load-deflection curve

does start with a vertical tangent, the tangent must become horizontal at points infinitely close to the origin. In other words, the slope variation near the origin is a Dirac delta function. From the physical viewpoint, what matters is the quadratic norm of the difference between the load-deflection curve and formula (29), and this norm approaches 0 if $D \to 0$. The behavior is sketched by the sequence of the dashed curves in Fig. 2b.

7. Asymptotic-matching approximation

The theory of Gao et al. (1999a, b) characterizes the deviation from the classical plasticity when the structure size D becomes too small. But this formulation has only a one-sided asymptotic support (on the scale of $\log D$). Ideally, one should seek a theory with a two-sided asymptotic support, having also realistic properties for the small-scale limit.

Smooth formulations with such two-sided asymptotic support are generally called the asymptotic matching. The earliest example is Prandtl's boundary layer theory in fluid mechanics. In solid mechanics, approximate formulae of the asymptotic matching type have met with considerable success in describing the size effects in quasibrittle materials such as concrete, rock, fiber composites and ice (e.g., Bažant and Planas, 1998; Bažant, 1997). Formulae of the asymptotic matching type are approximately applicable over the entire size range and have the potential of being generally more accurate than formulae having only a one-sided asymptotic support, as amply demonstrated by studies of concrete.

Even though the small-size asymptotic behavior lies outside the range of validity of Gao et al.'s (1999a, b) theory, we may use it to illustrate how to set up a simple asymptotic matching formula. Based on the established asymptotic properties, the broad-range transitional scaling law having both the classical macroscale plasticity and the gradient plasticity on the microscale as its asymptotes should be approximately describable by a smooth function approaching (21) for $D/l_\varepsilon \to 0$ and $\sigma_N = \text{constant}$ for $D/l_\varepsilon \to \infty$. This can be achieved by several simple formulae, and one of them is,

$$\sigma_N = \sigma_0 \left[1 + \left(\frac{D_0}{D} \right)^{2s/r} \right]^{r/2}, \quad s = 2 + \frac{p}{q}, \quad \sigma_0 = \alpha_0 \sigma_Y \chi \lambda_1^{p/q}, \quad D_0 = \alpha_0^{-1/s} l_\varepsilon, \tag{31}$$

(Fig. 2 top) where α_0 and r are dimensionless constants which need to be determined either experimentally or by a numerical solution of the boundary value problem of gradient plasticity for a suitable intermediate size D. In the plot of $\log \sigma_N$ versus $\log D$ (Fig. 2 top), the transitional size D_0 represents the intersection of the straight large-size and small-size asymptotes, and r determines the value of σ_N at $D = D_0$. Formula (31) has the advantage that a transformation of variables σ_N and D can reduce it to a linear regression plot. A similar approach can be used to construct an asymptotic matching formula once an improved theory with a more realistic small-size asymptotic behavior is formulated.

The small-size asymptotic behavior can of course be approached only at very small dimensions D which may well lie below the limit of applicability of a continuum

theory. Does that make the small-size asymptotic properties useless? Not really. The main purpose of knowing these properties is the asymptotic matching, which is the avenue leading to approximate formulae for the middle range. In this regard, it is important that the asymptotic behaviors at the extremes of the theory would not be totally unreasonable even if the theory does not apply at these extremes.

In this respect, the experience with the studies of scaling in concrete is worth noting. The size effect law for materials such as concrete has an inclined large-size asymptote corresponding to LEFM and a horizontal small-size asymptote corresponding to the theory of plasticity (Bažant and Planas, 1998). For many structure types, the small-size asymptote is closely approached only for structure sizes smaller than the size of mineral aggregates in concrete. Structures of such a size are hypothetical and cannot be produced. In spite of that, the formula with this kind of two-sided asymptotic support gives a very good description of the size effect in the range of realistic structure sizes.

8. Evaluations of tests of micro-torsion and micro-hardness

One case for which an explicit formula in terms of an integral has been obtained is the circular fiber of radius D subjected to torque T; see Eq. (35) in Huang et al. (1999). After transformation to dimensionless coordinates, that formula (for $p=1$ and $q=\frac{1}{2}$) reads:

$$\sigma_{\mathrm{N}}=\frac{T}{D^3}=\sigma_{\mathrm{Y}}\frac{2\pi\bar{\kappa}}{3}\int_0^1\left\{\frac{\bar{\sigma}}{\bar{\varepsilon}}\left(\rho^2+\frac{l_\varepsilon^2}{12D^2}\right)+\frac{l_\varepsilon^2 f(\bar{\varepsilon})f'(\bar{\varepsilon})}{12D^2\bar{\sigma}}\right\}\rho\,\mathrm{d}\rho, \tag{32}$$

where $\bar{\kappa}=\bar{\eta}=\kappa D=$ dimensionless specific angle of twist, $\kappa=$ actual specific angle of twist (rotation angle per unit length of fiber). By taking the limit of $\sigma_{\mathrm{N}}D^{5/2}$ for $D\to 0$, with σ_{N} given by the foregoing expression, one may readily check that the small-size asymptotic form of this formula is,

$$\sigma_{\mathrm{N}}=\sigma_{\mathrm{Y}}\left(l_\varepsilon^{5/2}\sqrt{\lambda_1}\frac{\pi}{18}\int_0^1\frac{\rho}{\bar{\varepsilon}}\,\mathrm{d}\rho\right)\bar{\kappa}^{3/2}D^{-5/2}, \tag{33}$$

which verifies our previous result (21), as well as (29) ($\bar{\kappa}$ plays the role of $\hat{w}$).

By optimal fitting of Eq. (31) to (32), one could obtain parameters D_0, σ_0 and r appropriate for the case of torsion. Gao et al. (1999b, in their Fig. 6), compared Eq. (32) to the results obtained from micro-torsion tests of fibers of diameters ranging from 12 to 170 μm. They achieved good agreement, except that the predicted stress-deformation curve for the smallest size was rising at about double the slope of the data. Generally, the stress corresponding to small deflections is underpredicted, and the stress corresponding to large deflections is overpredicted in Gao et al.'s theory. This systematic mismatch might be a manifestation of a transition to the locking response that characterizes the small-scale asymptotic behavior according to Eq. (21).

Gao et al. (1999b) have further noted that the test results for Rockwell microhardness tests of copper can be well approximated as

$$\sigma_{\mathrm{N}}=H_0\sqrt{A+\frac{h^*}{D}}, \tag{34}$$

(Fig. 2 top) where H_0 and h^* are constants and σ_N now stands for the hardness (stress average over the indentation area, denoted by Gao as H) and D is taken as the depth of penetration of the diamond cone (denoted by Gao as h). This test has the advantage that the situations at different depth of penetration of the cone are self-similar.

For small D, the foregoing formula has the asymptotic behavior $\sigma_N \approx \sqrt{h^*/D}$, which apparently contradicts our results in Eq. (21). A closer look, however, suggests that there need not be any contradiction. The test data used were of a limited size range, ranging from 0.15 to 6 μm. This testing range might be too narrow to completely characterize the size effect. The transition from the large-size to the small-size asymptotic behavior might be taking place over the range of D as wide as that from 0.01 to 100 μm.

In the plot of $\log \sigma_N$ versus $\log D$, the asymptotic matching formula has a slope gradually decreasing from $-\frac{5}{2}$ (if $p/q = \frac{1}{2}$) at $D = 0.005$ μm to 0 at $D = 100$ μm. It is possible that, within the aforementioned range of the micro-hardness tests of copper, the size effect curve has the slope of about $-\frac{1}{2}$ (Fig. 2 top), matching the size effect measured in these tests.

9. Simple modifications achieving reasonable asymptotic properties

It is easy to see that, as long as the third-order stresses τ_{ijk} are present in the differential equation of equilibrium (which occurs when the free energy density is a function of the strain gradient tensor or η), the small-size asymptotic behavior will have the kind of odd properties that have been demonstrated. Thus a more fundamental modification of the theory of Gao et al. (1999b) seems appropriate. With this motivation, let us explore here at least two simple modifications, leaving for future studies the difficult question as to whether such modifications can be physically justified by the theory of dislocations.

Modification I: Consider first the special case of Gao et al.'s (1999a) mathematical formulation in which l_ε is assumed to be negligible compared to l. According to Eqs. (2) and (15), the third-order stresses τ_{ijk} (and thus also $\bar{\tau}_{ijk}$) vanish. Then the strain gradient influences only the strain hardening and the dimensionless differential equations of equilibrium (17) take the standard form, with no third-order stresses. By the same procedure as before, these equations can be rearranged to the following dimensionless form:

$$\partial_i \frac{1}{\bar{\varepsilon}} \bar{\eta}^{p/q} \bar{\varepsilon}'_{ik} + \chi \bar{f}_k = 0, \quad \chi = \frac{\sigma_N}{\sigma_Y} \left(\frac{D}{\lambda_0} \right)^{p/q}. \tag{35}$$

In the same way as before, we conclude that, for geometrically similar structures, χ must be constant. The foregoing expression for χ yields the scaling law:

$$\sigma_N = \sigma_Y \left(\frac{\lambda_0}{D} \right)^{p/q}. \tag{36}$$

The asymptotic behavior of Eq. (34) based on micrometer-scale tests of Rockwell hardness (see Fig. 1 in Gao et al., 1999a or Fig. 5 in Gao et al., 1999b) is $\sigma_N \propto D^{-1/2}$ (which happens to be the same as the asymptotic behavior of the Hall–Petch formula

for the crystal size effect on metal strength, and the same as the size effect in linear elastic fracture mechanics). If $p/q = 1/2$ in Eq. (36), it would mean that the small-size asymptotic behavior is approached in microhardness tests when the indentation depth is about 0.1 μm. If $p/q = 1$, it would mean that the microhardness tests with the indentation depths around 1 μm are in about the middle of the transition between the opposite asymptotic behaviors.

Consider now the previously discussed special case in which all the dimensionless displacements $\bar{u}_k$ at all the points of similar structures increase in proportion to a parameter w such that $\bar{u}_k = w\hat{u}_k$ where $\hat{u}_k$ is not only independent of D but also invariable during the proportional loading process. By the same procedure as before, we obtain, instead of (20),

$$\partial_i \left(\frac{1}{\bar{\varepsilon}} \hat{\eta}^{p/q} \right) + \hat{f}_k = 0, \quad \text{with } \hat{f}_k = \frac{f_k}{c_1} w^{-p/q}, \quad c_1 = \sigma_Y \lambda_0^{p/q} D^{-(1+p/q)}. \tag{37}$$

From the foregoing field equation it now follows that if the relative displacement distribution (profile) $\hat{u}_k$ is constant during the loading process, as in torsion of a long cylinder, then the distribution $\hat{f}_k$ at the small-size limit must be constant as well. Using (37), we see that,

$$f_k = c_1 \hat{f}_k w^{p/q}, \tag{38}$$

where $c_1 \hat{f}_k$ is constant during loading. There are now two possibilities: (1) $p/q = 1$, in which case the load-deflection curve is a straight line; or (2) $p/q \neq 1$, in which case the initial stiffness (i.e., the slope of the initial tangent of the load-deflection curve) is either zero or infinite. The latter case is patently unreasonable. The former is not, but it is not quite realistic either because it does not permit modeling the inelastic behavior and failure.

Modification II: Second, consider again that the third-order stresses are absent (i.e., $l_\varepsilon \to 0$) but the strain gradient influences the argument of the plastic hardening function f. In particular, we consider (8) to be replaced by,

$$\frac{\sigma}{\sigma_Y} = f(\xi), \quad \xi = \bar{\varepsilon} + \frac{l}{D}\bar{\eta}. \tag{39}$$

For the hardening function $f(\xi)$ we choose the Ramberg–Osgood formula, which defines the inverse function $f^{-1}(\sigma)$ simply as,

$$\xi = f^{-1}\left(\frac{\sigma}{\sigma_Y}\right) = k_0 \frac{\sigma}{\sigma_Y} + k_1 \left(\frac{\sigma}{\sigma_Y}\right)^s, \tag{40}$$

where $k_0, k_1, s =$ positive constants, and $s > 1$. When the stresses are very small and D/l is very small as well, then,

$$\frac{\sigma}{\sigma_Y} = \frac{\xi}{k_0} = \frac{l}{k_0 D}\bar{\eta} \quad \text{or } \sigma \propto \bar{\eta}. \tag{41}$$

When the stresses are very high while D/l is again very small, then

$$\frac{\sigma}{\sigma_Y} = \left(\frac{\xi}{k_0}\right)^{1/s} = \left(\frac{l}{k_0 D}\bar{\eta}\right)^{1/s} \quad \text{or } \sigma \propto \bar{\eta}^{1/s}, \tag{42}$$

where $\propto$ is the proportionality sign. Except for the meaning of the proportionality constant, the last two equations are special cases of (36), with p/q replaced by 1 or by $1/s$. Therefore, by analogy with Eq. (38), the load-deflection curves in these asymptotic cases are as follows:

$$\text{for small } \sigma/\sigma_Y \text{ and small } D/l: \quad f_k \propto w \tag{43}$$

$$\text{for large } \sigma/\sigma_Y \text{ and small } D/l: \quad f_k \propto w^{1/s} \ (s > 1). \tag{44}$$

It follows that, in this modification, the small-size asymptotic load-deflection curve starts as a straight line of a finite slope and then, with a gradually decreasing slope, approaches a concave power curve (Fig. 2). From the phenomenological viewpoint, there is nothing strange about such a kind of asymptotic behavior.

Consequently, modification II seems to be more realistic, provided that it can be reconciled with the dislocation theory by logical arguments of the kind shown by Gao et al. (1999b). Investigation of this question is beyond the scope of this work and is left for subsequent studies.

The asymptotic matching approximation for this modification may again be taken in the form of Eq. (31), but with the exponent $s = 1$.

Finally, it should be emphasized that the small-size asymptotic properties of other theories of strain-gradient plasticity of metals on the micrometer scale have not been analyzed, except for the theory of Fleck and Hutchinson (1997). For that theory, it is found that the diagram of nominal torsional stress versus the specific angle of twist has a gradually decreasing slope for both the very large and very small ratios of the diameter to the characteristic length.

10. Conclusions

1. The experimental verification of the theory recently proposed by Gao et al. has so far been confined to the micrometer scale. An extension to smaller scales is not necessarily justified by the available experimental evidence.
2. The existing theory of gradient plasticity has only a one-sided asymptotic support, limited to the large-size asymptotic behavior. Its small-size asymptotic behavior is characterized by (1) a power scaling with exponent $-\frac{5}{2}$, which seems strangely high, and (2) an asymptotic approach to a load-deflection diagram whose tangent stiffness is initially zero and then gradually increases, as in locking materials. Such asymptotic behavior does not seem very realistic. A transition to such behavior might be the reason why Gao et al.'s theory appears too soft for small deflections and too stiff for large deflections.
3. It seems desirable to modify the theory so as to achieve a realistic two-sided asymptotic support.
4. A reasonable two-sided asymptotic behavior, matching the small-scale size effect observed in the tests of Rockwell hardness on the micrometer scale, can be achieved if the strain gradients are assumed to do no work and are considered to affect the plastic hardening function through a scalar parameter.

5. Whether such a kind of modification of the theory can be justified by extending experiments to still smaller sizes, whether it can be reconciled with the theory of dislocations, and whether it is the only way to avoid strange asymptotic properties, remain open questions. They are relegated to subsequent studies.
6. Other theories of gradient plasticity have not been analyzed, except that the previous theory of Fleck and Hutchinson was found to exhibit reasonable torsional response for both very large and very small wire diameters.

Acknowledgements

Partial support under U.S. National Science Foundation Grant CMS-9732791 to Northwestern University is gratefully acknowledged. Thanks are due to Milan Jirásek of EPFL, Lausanne, for pointing out that, even asymptotically for very small D, the load-deflection curve starts with a vertical slope, and to Zaoyang Quo of Northwestern University for pointing out the exceptional asymptotic scaling for pure bending.

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52 (2004) 975

JOURNAL OF THE MECHANICS AND PHYSICS OF SOLIDS

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Erratum

Erratum to "Scaling of dislocation-based strain-gradient plasticity" [Journal of the Mechanics and Physics of Solids 50 (2002) 435–448]☆

Zdeněk P. Bažant*

Department of Civil and Environmental Engineering, McCormick School of Engineering and Applied Science, Northwestern University, 2145 Sheridan Road, Evanston, IL 60208-3109, USA

An error exists in the treatment of the tensor function Φ_{ijk}. Similar to Λ_{ijk} and Π_{ijk}, the variable Φ_{ijk} as a function of deflection parameter w was considered in Eq. (27) to be a homogeneous function of degree 1. However, a dependence on w of the strain intensity $\bar{\varepsilon}$ appearing in the denominator of Eq. (3) was overlooked. This means that Φ_{ijk} is actually asymptotically independent of w. This correction affects Eqs. (28) and (30) in an obvious way, and the important consequence is that Eq. (29) should read $\bar{f}_k \propto c_0 w^{p/q}$ instead of $\bar{f}_k \propto w^{1+p/q}$. This further means that, for Gao et al.'s MSG theory, the initial load–deflection curve is $\bar{f}_k \propto w^{1/2}$ instead of $\bar{f}_k \propto w^{3/2}$, that the twist angle dependence in Eq. (33) should be $\bar{\kappa}^{1/2}$ instead of $\bar{\kappa}^{3/2}$, and that the curve at bottom left of Fig. 2 should be concave rather than convex. The main conclusions, which concern the scaling of nominal stress σ_N (including the excessive small-size asymptotic size effect), remain unaffected by this correction. Finally, in the sentence just before Section 5, replace the word 'enviously' by 'strangely'.

☆ doi of original article: 10.1016/S0022-5096(01)00082-5

* Corresponding author. Tel.: +1-847-491-4025; fax: +1-847-467-4011.
E-mail address: z-bazant@northwestern.edu (Z.P. Bažant).

doi:10.1016/j.jmps.2003.08.002