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On the gradient approach – Relation to Eringen's nonlocal theory

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ABSTRACT

A.C. Eringen has been a most active advocate of the nonlocal theory of continua finding many applications for it in solid, fluid, and electromagnetic media. His work is also used extensively for interpreting deformation and fracture phenomena at the micron and nano scales for which the gradient approach is also being used. The present paper is dedicated to Cemal's memory. It provides an account of the author's gradient approach as applied to elastic and plastic deformations with emphasis on ultrafine grain (ufg) and nanocrystalline (nc) polycrystals, also in comparison with the nonlocal theory. The results reported herein have been strongly motivated by Eringen's works and vision, as well as by his example of endurance and kindness.

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1. Introduction

In two previous papers published 18 years ago in a Special Issue of this Journal dedicated to Eringen on the occasion of his 70th birthday generalized models of continua were formulated and solutions to specific problems were obtained to interpret experimental observations that could not be captured by classical theory. One paper by the author (pp. 1279–99) illustrated how gradient dependent constitutive equations can lead to the determination of shear band widths/spacings and the elimination of elastic strain singularities that occur during deformation localization and fracture. Another paper by Eringen (pp. 1551–65) was much broader in scope illustrating how nonlocal or integral type constitutive equations can provide new input not only for deformation and fracture, but also for other problems of fluid mechanics and electromagnetic theory.

The common basic premise in both papers was the introduction of a characteristic material parameter or internal length to account either for the effect of underlying microstructure in complex media, or the interaction of "bulk" and "surface" points in small size volumes. While Eringen's approach appeared to be more general in its formulation, its application to dislocation and crack problems resulted eventually to a reduced constitutive equation incorporating the Laplacian of stress in the standard linear expression of Hooke's law. On the contrary, the author's starting point for elasticity problems was the generalization of classical Hooke's law by an extra term containing the Laplacian of strain. As a result, stress singularities were eliminated in the first case, while strain singularities were eliminated in the second case. [In fact, for a screw dislocation, the nonsingular expression for the stress in the first case turned out to be the same with the nonsingular expression for the strain (within a multiplicative shear modulus factor) in the second case.]

However, microscopic heterogeneity in both stress and strain is usually developed during elastic or plastic deformations and, therefore, both stress and strain gradients should be accounted for in the relevant constitutive equations leading to the description of a larger class of deformation and fracture phenomena. A formal justification for such type of stress and/or strain gradient dependencies for elasticity and plasticity is provided in Section 2 by introducing the concept of implicit gradient constitutive equations.

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In Section 3, gradient dependent stress–strain relations for elastic and plastic deformations at the micron and submicron regimes are derived by viewing the continuum as a medium where its (bulk) points can exchange momentum with internal or external surfaces. As a result, a nonlocal source term appears in the momentum balance and higher order gradients are generated in the governing differential equations depending on the constitutive assumptions made for this extra term. The simple original models of gradient elasticity and gradient plasticity discussed in Section 2 can now be derived within this bulk–surface interaction approach. These micro/nano elasticity and micro/nano plasticity constitutive equations can conveniently be extended to include rate effects and nonlinearities. The resulting equations can be used for interpreting viscoelastic and viscoplastic behavior at the micro/nano scales and discuss, in particular, strain or strain rate softening instabilities along with corresponding phenomena of nucleation/propagation of strain or strain rate bands. Such gradient dependent rate equations can alternatively be derived by focusing, instead of the momentum balance, to a mass balance equation taking into account the exchange of "effective" mass between bulk and surface points which takes place through the carriers of anelastic or plastic deformation, such as vacancies, dislocations, and other structural defects.

In Section 4 three basic problems are considered within the gradient approach. The first problem is concerned with the elimination of elastic singularities from crack tips as this topic was Eringen's favored one. The second problem is concerned with the derivation of a modified version of Johnson's spherical cavity model for indentation within a simple gradient plasticity framework. The third problem is concerned with nucleation and growth of strain bands; in particular, the propagation of a deformation front as a result of the competition between deterministic gradients and stochastic effects, and the manifestation of this phenomenon in the serrated stress–strain graph. Finally, in Section 5 certain results on size dependent stress–strain curves obtained for nanopolycrystals of varying grain size are presented. The experimental curves are again interpreted through gradient dependent constitutive equations where, however, the gradient term is now replaced by a grain size dependent term derived on the basis of a simplified dimensional but robust microscopic argument.

2. Implicit gradient constitutive equations

2.1. Gradient elasticity

In general, both strain and stress gradients may affect the constitutive response of materials. A systematic way to account for this is to employ the framework of implicit constitutive equations (Morgan, 1966; Rajagopal & Srinivasa, 2009). In the case of gradient dependent elasticity models, this idea may most simply be pursued by starting with an implicit constitutive equation of the form

$$\mathbf{f}(\boldsymbol{\sigma}, \boldsymbol{\varepsilon}, \nabla^2\boldsymbol{\varepsilon}, \nabla^2\boldsymbol{\sigma}) = 0, \tag{1}$$

where $\mathbf{f}$ is a general linear isotropic function of both stress and strain, as well as of their Laplacians. It is pointed out that the dependence of the first gradients $\nabla\boldsymbol{\varepsilon}$, $\nabla\boldsymbol{\sigma}$ is suppressed as this would lead, in general, to third order tensors that previous linear models of gradient elasticity do not usually consider. There might be, however, situations where the first gradients need to be accounted for, like in the case of beam bending within an approximate strength of materials treatment. In this case the second gradient of strain vanishes and related size effects have been interpreted by assuming that the axial stress depends on the strain and its first gradient (Aifantis, 1999).

In the special case when $\mathbf{f}$ in Eq. (1) is a linear isotropic tensor function of its arguments, the relevant representation theorem for $\mathbf{f}$ gives

$$\mathrm{tr}(\alpha_1\boldsymbol{\varepsilon} + \alpha_2\boldsymbol{\sigma})\mathbf{1} + \alpha_3\boldsymbol{\varepsilon} + \alpha_4\boldsymbol{\sigma} + \nabla^2[\mathrm{tr}(\alpha_5\boldsymbol{\varepsilon} + \alpha_6\boldsymbol{\sigma})\mathbf{1} + \alpha_7\boldsymbol{\varepsilon} + \alpha_8\boldsymbol{\sigma}] = 0, \tag{2}$$

where the coefficients α's are constants. Various strain and/or gradient models that have previously appeared in the literature can be obtained by properly selecting the constants α's.

In this connection, it is pointed out that the models corresponding to non-vanishing α_6 and α_8 are not contained in Mindlin's strain gradient theory (e.g. Mindlin & Eshel, 1968 and references quoted therein). In particular, the following gradient models may be obtained on the basis of Eq. (2) through a proper choice of the constants α's

$$\sigma_{ij} = C_{ijkl}(1 - c\nabla^2)\varepsilon_{kl}; \quad \varepsilon_{ij} = C^{-1}_{ijkl}(1 - c\nabla^2)\sigma_{kl}; \quad (1 - c_1\nabla^2)\sigma_{ij} = C_{ijkl}(1 - c_2\nabla^2)\varepsilon_{kl}, \tag{3}$$

where C_{ijkl} is the usual fourth-order elastic stiffness tensor which in the isotropic case is expressed in terms of the Lamé constants (λ, μ) as $C_{ijkl} = \lambda\delta_{ij}\delta_{kl} + \mu(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk})$. The model of Eq. $(3)_1$ is the one used by Aifantis and co-workers (e.g. Aifantis, 1992; Altan & Aifantis, 1997; Askes, Bennett, Gitman, & Aifantis, 2008; Exadaktylos, Vardoulakis, & Aifantis, 1996; Gutkin & Aifantis, 1999; Lazar, Maugin, & Aifantis, 2005; Ru & Aifantis, 1993; Unger & Aifantis, 1995) to eliminate strain singularities and interpret size effects; as well as several other authors (e.g. Georgiadis, 2003; Karlis, Tsinopoulos, Polyzos, & Beskos, 2007; Stamoulis & Giannakopoulos, 2008), often without proper references. The model of Eq. $(3)_2$ is the one derived by Eringen on the basis of a nonlocal relation between stress ($\boldsymbol{\sigma}$) and strain ($\boldsymbol{\varepsilon}$) (e.g. Eringen, 1977, 1983, 1985, 1992, 2002; Eringen, Speziale, & Kim, 1997). The model in Eq. $(3)_3$ is an example of implicit gradient elasticity. It was discussed by the author in Aifantis (2003) and has been shown (in contrast to Eq. $(3)_1$ which leads to the elimination of strain singularities and to Eq. $(3)_2$ which leads to the elimination of stress singularities) that it can eliminate both strain and stress singularities from dislocation lines and crack tips (e.g. Aifantis, 2009a, 2009b and references quoted therein).

An alternative derivation of the implicit gradient elasticity model given by Eq. $(3)_3$ may be established by starting with Eringen's nonlocal model (see, for example, Eringen, 1983, 1985, 1992)

$$\sigma_{ij} = \int_\Omega k(|x-x'|)(\lambda\varepsilon^c_{kk}(x')\delta_{ij} + 2\mu\varepsilon^c_{ij}(x'))\,d\Omega; \quad k(x-x') = \frac{c_1}{2\pi}K_0\left(c_1\sqrt{(x-x')^2+(y-y')^2}\right), \tag{4}$$

where K_0 denotes modified Bessel function. It then follows (Altan & Aifantis, 1997), through a Taylor expansion up to second order terms, that $\sigma_{ij} - c_1\nabla^2\sigma_{ij} = \sigma^c_{ij}$ with $\sigma^c_{ij} = \lambda\varepsilon^c_{kk} + 2\mu\varepsilon^c_{ij}$; i.e. $(\boldsymbol{\sigma}^c, \boldsymbol{\varepsilon}^c)$ denotes a classical local Hookean pair of stress and strain fields related through the standard linear elasticity expression. By using the definition of a "macroscopic" strain tensor ε_{ij} as a volume-type average of the local strain tensor ε^c_{ij}, i.e. $\varepsilon_{ij}(\mathbf{x}) = (1/V_\Omega)\int_\Omega \varepsilon^c_{ij}(\mathbf{x}+\mathbf{r})d\Omega$ and expanding in a Taylor series up to second order terms as before, it can be shown (Aifantis, 1995) that $\varepsilon_{ij} = \varepsilon^c_{ij} + c_2\nabla^2\varepsilon^c_{ij}$. The positive constant c_2 depends on the size of the elementary volume ($\propto R^2/10$ for a spherical volume V_Ω of radius R) which, in turn, depends on the underlying microstructure and the degree of existing heterogeneity. The preceding expression can be inverted, within a second spatial order approximation (e.g. Vardoulakis & Aifantis, 1989), to read $\varepsilon^c_{ij} = \varepsilon_{ij} - c_2\nabla^2\varepsilon_{ij}$; and, thus, the above relation between σ_{ij} and σ^c_{ij} is reduced to the model of Eq. $(3)_3$ for isotropic C_{ijkl}. [A similar argument for Eq. $(3)_3$ was first advanced in Aifantis (2010) where a typo ($c_2 \propto 1/R^2$ instead of $c_2 \propto R^2/10$) has occurred.]

Another yet more general derivation, but with a different interpretation of Eq. $(3)_3$ may be obtained by a slight modification of a "homogenization" argument utilized in Gitman, Askes, and Aifantis (2005). Instead of writing an integral expression for the "macroscopic" stress σ^M_{ij} by viewing it as a volume average of the "microscopic" stress σ^m_{ij} and assuming a linear inhomogeneous relation for it in terms of the microscopic strain ε^m_{ij} (Gitman et al., 2005), we introduce an average stress Σ_{ij} and an inhomogeneous scale modulus H_{ijkl} such that $\Sigma_{ij} = (1/V^\Sigma_{RVE})\int_{V_{RVE}} H^\Sigma_{ijkl}\sigma^\Sigma_{kl}\,dV$. The quantity V^Σ_{RVE} denotes the elementary representative volume over which the average stress Σ_{ij} is calculated or measured, and the scale modulus H^Σ_{ijkl}, as well as the local stress field σ^Σ_{ij}, vary within V^Σ_{RVE}. Next, we assume linear Taylor expansions of the form $H^\Sigma_{ijkl} = H_{ijkl} + H^\Sigma_{ijkl,m}\delta x_m$ and $\sigma^\Sigma_{ij} = \sigma_{ij} + \sigma^\Sigma_{ij,m}\delta x_m$, where H_{ijkl} and σ_{ij} are the values of H^Σ_{ijkl} and σ^Σ_{ij} at the center of the assumed elementary volume, say a cube, of characteristic size ℓ. By carrying then out the integration in the above equation for Σ_{ij}, it can be shown that $\Sigma_{ij} = H_{ijkl}[\sigma_{kl} - (\ell^2/12)\sigma_{kl,mm}]$; and a similar expression can be deduced for an average strain E_{ij}, if the same scale modulus is assumed and the same size is also considered for the representative elementary volume over which the local strain is integrated. Finally, on assuming that the average stress Σ_{ij} is linearly related to the average strain E_{kl} by an average constant stiffness $C_{ijkl}(\Sigma_{ij} = C_{ijkl}E_{kl})$, the model of Eq. $(3)_3$ is deduced with $c_1 = c_2$. [Different values of c_1 and c_2 are obtained if the scale moduli H^Σ_{ijkl} and H^E_{ijkl} and the corresponding representative elementary volume sizes ℓ^Σ and ℓ^E are different for the stress and strain fields. It is also noted that, for notational convenience, throughout this paper the same symbol c is used sometimes for gradient terms of different form and meaning, as well as sign.]

In concluding this subsection on gradient elasticity, it is noted that another special model – more general, however, than the isotropic version of Eq. $(3)_1$ – of the general case of Eq. (2) may be deduced by assuming $\alpha_1 \neq \alpha_5$ (both $\neq 0$) and $\alpha_2 = \alpha_6 = \alpha_8 = 0$. Then by writing out explicitly the corresponding equilibrium equation in terms of the displacement $\mathbf{u}$, the result is

$$(\lambda+\mu)(1 - c*\nabla^2)\operatorname{div}\mathbf{u} + \mu(1 - c\nabla^2)\nabla^2\mathbf{u} = 0, \tag{5}$$

where (c^*, c) are directly related to α's in Eq. (2). For $c = c^*$ this model is reduced to that of the isotropic version of Eq. $(3)_1$; otherwise, Eq. $(3)_1$ is generalized, as it should, to include two different gradient coefficients for the hydrostatic and shear gradient contribution. The above model with $c = 0$ has been used earlier to interpret size effects in hollow specimens (e.g. Aifantis, 1999, 2009a, 2010 and references quoted therein).

2.2. Three critical remarks on the original gradient elasticity model (GRADELA)

2.2.1. The robustness of GRADELA

The GRADELA model, i.e. the isotropic version of Eq. $(3)_1$, is the simplest possible case of strain gradient elasticity incorporating both volumetric and shear effects. This model was initially derived for elastically deforming nanopolycrystals viewed as a mixture of two phases: the "bulk" and the "grain boundary" phases, each supporting their own displacement and Hookean stress fields, and interacting with each other through an internal body force proportional to the relative displacement (see, for example, Aifantis, 1994; Altan & Aifantis, 1997 and references quoted therein). This was certainly a different motivation than the one led Mindlin (Mindlin & Eshel, 1968) to a substantially more involved strain gradient elasticity theory by assuming the most general quadratic dependence of the elastic energy density on the first gradients of the strain tensor, as it will be discussed below. The main advantage of GRADELA, (which contains only one extra constant) over Mindlin's theory (which contains five extra constants) is the fact that solutions of boundary value problems can be found in terms of corresponding solutions of classical elasticity through an inhomogeneous Helmholtz equation (Ru–Aifantis theorem; Ru & Aifantis, 1993). This is partly why the interest in gradient elasticity has been revived in recent years following the publication of the original robust GRADELA model in the mid nineties, as discussed in Aifantis (2010) and papers quoted therein. In this connection, the work of Sharma and co-workers (see, for example, Maranganti & Sharma, 2007 and the rest of his papers referenced therein) is mentioned as an example. He found many applications of gradient elasticity for various nanotechnology problems. He used a slightly more general version than GRADELA, but in our opinion, all his results could be obtained by using the isotropic version of Eq. $(3)_1$ with simpler solution formulae and without loss of physical insight or other pertinent information.

An additional point that is frequently overlooked by current workers on nonlinear elasticity with a non-convex strain energy density, has to do with the fact that GRADELA has indeed readily motivated the inclusion of strain gradients in this field. The first paper on this topic by Triantafyllidis and Aifantis (1986) was concerned with the localization of deformation in hyperelastic softening materials. Even though not widely recognized, this article has prompted a large amount of recent work on phase transitions (twinning and martensitic transformations) in modern continuum mechanics where the introduction of strain gradients in the non-convex form of strain energy function has provided a "stabilizing" mechanism for capturing spatial features of the evolving microstructural phases when the material enters the regime (non-convex region) where homogeneous states are unstable.

2.2.2. Relation to Mindlin's theory

Another clarifying remark concerns the relation of GRADELA to Mindlin's strain gradient elasticity theory (Mindlin & Eshel, 1968). Mindlin's starting point is a strain energy density expression of the form

$$w = w^c + c_1 \varepsilon_{ij,j}\varepsilon_{ik,k} + c_2 \varepsilon_{ii,k}\varepsilon_{kj,j} + c_3 \varepsilon_{ii,k}\varepsilon_{jj,k} + c_4 \varepsilon_{ij,k}\varepsilon_{ij,k} + c_5 \varepsilon_{ij,k}\varepsilon_{kj,i}, \tag{6}$$

where the first term w^c of the rhs is the classical Hookean contribution and the rest five terms comprise the most general contribution of the first gradients of the strain tensor. In this notation, the corresponding strain energy density expression for GRADELA reads

$$w = w^c + c/2\sigma^c_{ij,k}\varepsilon_{ij,k}; \quad 2w^c = \sigma^c_{ij}\varepsilon_{ij}; \quad \sigma^c_{ij} = \lambda\varepsilon_{mm}\delta_{ij} + 2\mu\varepsilon_{ij} \Rightarrow \sigma_{ij,j} = 0; \quad \sigma_{ij} = \sigma^c_{ij} - c\nabla^2\sigma^c_{ij}, \tag{7}$$

where the last two relations of Eq. (7) are deduced from a virtual work "principle" (Aifantis, 2010) similar to that of Mindlin's (Mindlin & Eshel, 1968). Mindlin defines an elastic second order stress $\sigma^c_{ij} = \partial w/\partial\varepsilon_{ij}$ and a third order stress $\tau_{ijk} = \partial w/\partial\varepsilon_{ij,k} = c\sigma^c_{ij,k}$ in our terminology, and derives boundary conditions from the aforementioned variational principle which, even in the simple case of GRADELA, are complicated in form and often difficult to interpret physically. In fact, the isotropic version of Eq. $(3)_1$ results form Mindlin's strain energy function given by Eq. (6) when the choice

$$c_1 = c_2 = c_5 = 0, \quad c_3 = \lambda c/2, \quad c_4 = \mu c, \tag{8}$$

is made. In this connection, it is noted that in Feynman's linear theory of gravity (Feynman, 1995) – see also the discussion by Lazar and Maugin (2005) contained in the reference for Feynman listed in the bibliography – an expression like Mindlin's given by Eq. (6) is used but the following choice is made for the gradient coefficients

$$c_1 = -c_2 = -2\mu c, \quad c_3 = -c_4 = -\mu c, \quad c_5 = 0. \tag{9}$$

Then it easily turns out that the quantity $(1/2\mu c)\tau_{ijk,k} = -(inc\varepsilon)_{ij} = \varepsilon_{ikl}\varepsilon_{jmn}\varepsilon_{\ln,km}$ is equivalent to the 3-D linear Einstein's tensor. Initially, gauge theories of dislocations (see, for example, Lazar & Anastassiadis, 2009 in the reference for Feynman listed in the bibliography and references therein) were based on Feynman/Einstein choice of the constants c's given by Eq. (9), but they gave unphysical results; the situation was repaired afterwards by essentially employing Aifantis' choice of c's given by Eq. (8), leading to the isotropic version of Eq. $(3)_1$. It is also important to point out here that the stress σ_{ij} satisfying the standard equilibrium equations is identified as the Cauchy stress for which boundary conditions should be assigned. In this connection, it is noted that in other recent articles (e.g. those by Lazar and co-workers; see references in the bibliography) a different terminology is used: σ^c_{ij} is referred to as the Cauchy stress and σ_{ij} is referred to as the total stress. This difference in interpretation is of no consequence in the present discussion and it will be elaborated upon elsewhere.

2.2.3. GRADELA's J-integral

Several results of elasticity theory concerning dislocations, cracks and other inhomogeneities can be extended within the GRADELA model. In particular, many expressions derived for dislocations by using linear elasticity can now be revisited with GRADELA to obtain corresponding scale-dependent expressions and re-interpreting related physical phenomena at small scales. For example, the appropriate expression for the J-integral is

$$J_k = \int_C [w\delta_{jk} - \sigma^c_{ij}u_{i,k} - c\sigma_{ij,l}u_{i,lk}]n_j \, dC, \tag{10}$$

where w denotes the appropriate gradient dependent elastic strain energy density (i.e. $2w = \sigma^c_{ij}\varepsilon_{ij} + c\sigma^c_{ij,l}\varepsilon_{ij,l}$; $\sigma^c_{ij} = \lambda\varepsilon_{mm}\delta_{ij} + 2\mu\varepsilon_{ij}$) and C is a closed curve surrounding, for example, the crack tip. The usefulness of the above expression in gradient elastic fracture mechanics has to be assessed; a task left for a future article where the Peach–Koehler force, the image force, and other key-formulae of classical dislocation theory will be revisited and their implications to various engineering configurations at the nanoscale will be discussed. Finally, it is noted that the simple formula given by Eq. (10) can also be deduced from the rather complex mathematical expressions derived recently by Lazar and co-workers for conservation laws of more general gradient elasticity theories (Agiasofitou & Lazar, 2009).

2.3. Gradient plasticity

Next, attention is focused to deformation theory of plasticity for which the isotropic function **f** in the beginning of this section is replaced by a scalar isotropic function f designating the yield condition. A generalized yield condition can then be deduced (by using standard representation theorems for isotropic scalar functions) in terms of the invariants of (σ, ε) and their Laplacians. If a J_2-type gradient dependent yield condition is desirable, the corresponding yield expression for the case of isotropic hardening may be written as

$$\tau - c * \nabla^2\tau = \kappa(\gamma) - c\nabla^2\gamma, \tag{11}$$

where τ (the flow or equivalent stress) and γ (the equivalent plastic strain) are the second invariants of the deviatoric stress and plastic strain tensors; defined later after Eq. (19). For $c^* = 0$, Eq. (11) reduces to the author's original gradient plasticity model (Aifantis, 1984). Various justifications for the original ($c^* = 0$) gradient dependent yield condition (or gradient dependent flow stress) have been provided in previous articles (e.g. Aifantis, 1992, 1994, 1995, 2003 and references quoted therein) with a most recent account provided in Aifantis (2009b) and Forest and Aifantis (2010). In Aifantis (2009b) the $\nabla^2\gamma$ in Eq. (11), with $c^* = 0$, is derived from the configuration of single slip and a scale invariance argument by also averaging over all possible slip systems (Section 4 of Aifantis (2009b)). In Forest and Aifantis (2010) a link is established between Eringen's micromorphic theory and the author's gradient plasticity theory (Section 2.2 of Forest and Aifantis (2010)).

On returning to Eq. (11), it is remarked that the arguments employed earlier in this section for deriving various types of gradient elasticity models can also be adapted to the case of plasticity. In this connection it is pointed out that if first gradients are included in the general form of the yield condition discussed above, the following expression may be deduced

$$\tau - \bar{c}^*\nabla\tau\cdot\nabla\tau - c^*\nabla^2\tau = \kappa(\gamma) - \bar{c}\nabla\gamma\cdot\nabla\gamma - c\nabla^2\gamma. \tag{12}$$

This equation with $(c^* = \bar{c}^* = 0)$ was used earlier to interpret size effects in bending (Aifantis, 1999; Tsagrakis, Konstantinidis, & Aifantis, 2003).

3. Deformation in nanovolumes: the bulk–surface interaction

An extended continuum mechanics framework is outlined here for addressing the mechanical response of ultrafine grain (ufg) and nanocrystalline (nc) polycrystals. This extension is based on generalizing the standard continuum mechanics structure by introducing extra terms modeling the "interaction" between "bulk" and (external or internal) "surface" points, as well as appropriate constitutive equations for these terms. We apply this idea below to consider separately elastic and plastic deformations, and separately viscoelastic and viscoplastic deformations. Such "bulk–surface" interaction idea was first outlined in Aifantis (1978) where the standard balance laws for mass, momentum, energy and entropy where generalized to include nonlocal source terms accounting for the aforementioned exchange processes between bulk and surface points. The resulting governing differential equations are proposed to be used in connection with the determination of the mechanical response of polycrystals at the submicron and nano regimes for both elastic (micro/nanoelasticity) and plastic (micro/nanoplasticity), as well as viscoelastic (micro/nanoviscoelasticity) and viscoplastic (micro/nanoviscoplasticity) deformations.

3.1. Micro/nanoelasticity

Within the bulk–surface interaction approach the standard equilibrium equation div $\boldsymbol{\sigma} = 0$ is generalized to include an additional internal body force $\hat{\mathbf{f}}$ representing the exchange of momentum between bulk and surface, for the present case of small volumes. Then, the balance law of linear momentum in the absence of inertia effects reads

$$\operatorname{div}\boldsymbol{\sigma}^{\mathrm{B}} = \hat{\mathbf{f}}, \tag{13}$$

where $\boldsymbol{\sigma}^{\mathrm{B}}$ is the usual stress tensor of the bulk material and $\hat{\mathbf{f}}$ is an internal-like force modeling the momentum exchange between the "bulk" and "surface" points. It is further assumed that $\hat{\mathbf{f}}$ is determined by a higher-order stress or "hyperstress" M of third order which, in turn, may be expressed as the gradient of the second-order stress **S** or extra stress modeling bulk–surface interaction; i.e. $\hat{\mathbf{f}} = \operatorname{div}\operatorname{div}\mathsf{M};\ \ \mathsf{M} = \nabla\mathbf{S}$.

The simplest possible constitutive assumption for the extra stress **S** is to assume it proportional to the bulk stress $\boldsymbol{\sigma}^{\mathrm{B}}$, i.e. $\mathbf{S} = c\boldsymbol{\sigma}^{\mathrm{B}}$, and then Eq. (13) can be written as

$$\operatorname{div}\boldsymbol{\sigma} = 0; \quad \boldsymbol{\sigma} = \boldsymbol{\sigma}^{\mathrm{B}} - \nabla^2\boldsymbol{\sigma}^{\mathrm{B}}. \tag{14}$$

If for $\boldsymbol{\sigma}^{\mathrm{B}}$ we adopt the usual Hooke's law of classical elasticity, i.e. $\boldsymbol{\sigma}^B = \lambda(\mathrm{tr}\boldsymbol{\varepsilon})\mathbf{1} + 2\mu\boldsymbol{\varepsilon}$, where (λ, μ) denote, as before, the Lamé constants, it follows that the total stress $\boldsymbol{\sigma}$, including both the usual stress corresponding to the bulk and its interaction with the surface, is determined by the equation

$$\operatorname{div}\boldsymbol{\sigma} = 0; \quad \boldsymbol{\sigma} = \lambda(\mathrm{tr}\boldsymbol{\varepsilon})\mathbf{1} + 2\mu\boldsymbol{\varepsilon} - c\nabla^2[\lambda(\mathrm{tr}\boldsymbol{\varepsilon})\mathbf{1} + 2\mu\boldsymbol{\varepsilon}], \tag{15}$$

i.e. the equations of the original GRADELA model.

3.2. Micro/nanoplasticity

To derive modified equations for plasticity, attention should be focused first on the yield condition and the corresponding expression for the flow stress, as this is the starting point in any development of plasticity theory. This can be done, along similar lines as for the elastic case, by considering the case of simple shear for which the corresponding one-dimensional counterpart of Eq. (13) reads

$$\partial_y \tau^b = \hat{f}. \tag{16}$$

Here τ^b is the bulk shear stress and $\hat{f}$ is the one-dimensional scalar counterpart of the exchange of momentum force between "bulk" and "surface" points. In physical terms, τ^b may be identified with the resolved shear stress on a representative slip system with the coordinate x denoting the slip direction and y the coordinate normal to it. As in the elastic case, it is assumed that the scalar $\hat{f}$ is given by the second spatial derivative of another scalar field M which, in turn, is given by the spatial derivative of another scalar field S, i.e. $\hat{f} = \partial_{yy}M;\ M = \partial_y S$. Then Eq. (16) yields

$$\partial_y \tau = 0 \Rightarrow \tau = \tau^b - \partial_y M, \tag{17}$$

where the second equation may now be viewed as the appropriate gradient-dependent expression for the flow stress, required for continuous yielding. Unlike to the linear elastic case where the interaction of "bulk" and "surface" points can be expressed equivalently either in terms of stress or in terms of strain, it is assumed here that in the case of plastic flow it is the shear strain γ which determines the bulk–surface interaction. In other words, it is assumed that $S = c\gamma$ with c being a constant and, thus, Eq. $(17)_2$ can be written as

$$\tau = \kappa(\gamma) - c\partial_{yy}\gamma, \tag{18}$$

where the standard plasticity relation $\tau^b = \kappa(\gamma)$ was assumed for the bulk stress. The three-dimensional generalization of Eq. (18) reads

$$\tau = \kappa(\gamma) - c\nabla^2\gamma, \tag{19}$$

where τ is the equivalent or effective stress $\tau = \sqrt{1/2\sigma'_{ij}\sigma'_{ij}};\ \sigma'_{ij} = \sigma_{ij} - 1/3\sigma_{kk}\delta_{ij}$ and γ the corresponding equivalent or effective shear strain (i.e. $\gamma = \int \dot{\gamma}\,dt,\ \dot{\gamma} = \sqrt{2\dot{\varepsilon}_{ij}\dot{\varepsilon}_{ij}}$ with $\dot{\varepsilon}_{ij}$ denoting the rate of the plastic strain tensor).

Alternatively, for cases where stress gradients determine the bulk–surface interaction, the quantity S may be taken to be proportional to the bulk stress τ^b as in the elastic case. Then, the corresponding expression of the flow stress τ reads

$$\tau = \kappa(\gamma) - c\nabla^2\gamma - \bar{c}\nabla\gamma\cdot\nabla\gamma, \tag{20}$$

where the gradient coefficients are proportional to $\kappa'(\gamma)$ and $\kappa''(\gamma)$ respectively, with prime denoting differentiation of a function with respect to its argument. In other words, a special case ($c^* = \bar{c}^* = 0$) of the phenomenological implicit gradient constitutive expression given by Eq. (12) has resulted where, however, the internal length parameters (as determined by the gradient coefficients c and $\bar{c}$) vary with the plastic strain γ. Such types of gradient dependent flow stress have been used in Tsagrakis et al. (2003) to model size effects in microbending.

3.3. Rate effects

In this section it is shown how to include rate effects for deforming micro/nano volumes within the above framework. For viscoelastic behavior and a Kelvin–Voigt type solid this can easily be done on the basis of Eq. (13) of Section 3.1 by assuming that the bulk stress $\boldsymbol{\sigma}^{\mathrm{B}}$ is given by the standard expression

$$\boldsymbol{\sigma}^{\mathrm{B}} = \lambda(\mathrm{tr}\boldsymbol{\varepsilon})\mathbf{1} + 2\mu\boldsymbol{\varepsilon} + \lambda^*(\mathrm{tr}\dot{\boldsymbol{\varepsilon}})1 + 2\mu^*\dot{\boldsymbol{\varepsilon}}, \tag{21}$$

where the superimposed dot denotes time differentiation and (λ^*, μ^*) are the corresponding viscoelastic constants. Then, the arguments that led to Eqs. (14) and (15) can be adopted to derive, instead of Eq. $(15)_2$, the following gradient generalization of a Kelvin–Voigt solid

$$\boldsymbol{\sigma} = [\lambda(\mathrm{tr}\boldsymbol{\varepsilon})\mathbf{1} + 2\mu\boldsymbol{\varepsilon}] + [\lambda^*(\mathrm{tr}\dot{\boldsymbol{\varepsilon}})\mathbf{1} + 2\mu^*\dot{\boldsymbol{\varepsilon}}] - c\nabla^2[\lambda(\mathrm{tr}\boldsymbol{\varepsilon})\mathbf{1} + 2\mu\boldsymbol{\varepsilon}] - c^*\nabla^2[\lambda^*(\mathrm{tr}\dot{\boldsymbol{\varepsilon}})\mathbf{1} + 2\mu^*\dot{\boldsymbol{\varepsilon}}], \tag{22}$$

where the new gradient coefficient c^* measuring the effect of strain rate gradients may be neglected in a first approximation for solid-like behavior, but not for a fluid-like behavior. A similar procedure can be employed for a Maxwell type of viscoelastic behavior, as well as for more general viscoelastic responses of integral type.

A similar procedure can be followed for viscoplasticity by allowing the homogeneous part of τ^b to depend on $\dot{\gamma}$ and assuming that $\mathbf{S}$ varies linearly with $\dot{\gamma}$, in addition to γ. It easily follows then that the viscoplastic counterpart of Eq. (19) reads

$$\tau = \kappa(\gamma, \dot{\gamma}) - c\nabla^2\gamma - c^*\nabla^2\dot{\gamma}, \tag{23}$$

where in a first approximation for solid-like behavior the $c^*\nabla^2\dot{\gamma}$ term may be neglected. For linear viscous behavior (i.e. for $\kappa(\gamma,\dot{\gamma}) = \kappa(\gamma) + \eta\dot{\gamma}$, with η denoting viscosity), Eq. (23) reduces to $\tau = \kappa(\gamma) + \eta\dot{\gamma} - c\gamma_{yy}$ for one-dimensional strain softening problems for which $\kappa(\gamma)$ has a negative slope regime; $\kappa'(\gamma) < 0 \Rightarrow c > 0$. Alternatively, for linear hardening behavior but nonlinear rate effects [as in the case of Portevin-Le Châtelier (PLC) effect; Aifantis, 1992, 1984/1987] Eq. (23) reduces to $\sigma = h\varepsilon + f(\dot{\varepsilon}) - c\varepsilon_{xx}$ for one-dimensional strain rate softening problems for which $f(\dot{\boldsymbol{\varepsilon}})$ is a nonconvex function with a negative slope regime; $f'(\dot{\boldsymbol{\varepsilon}}) < 0 \Rightarrow c < 0$ ($\boldsymbol{\sigma}$ is the tensile stress, $\boldsymbol{\varepsilon}$ is the tensile strain and h is the hardening modulus). It is noted that the above constitutive equation for τ may be used for modeling the nucleation and propagation of shear bands (in the y-direction along which γ varies) for dynamic deformations when the material enters the stain softening regime for constant strain rate tests, while the constitutive equation for $\boldsymbol{\sigma}$ has been used for modeling the propagation of PLC bands (in the x-direction along which $\boldsymbol{\varepsilon}$ varies) for quasistatic deformations when the material enters the strain rate softening regime for constant stress rate tests.

An alternative way to include viscoplastic effects within the bulk–surface interaction framework is by utilizing – instead of the momentum balance given by Eq. (16) – an effective mass balance equation of the form

$$\dot{\rho}^{\mathrm{B}} + \mathrm{div}\,\mathbf{j}^{\mathrm{B}} = \hat{c}, \tag{24}$$

where ρ^{B} denotes the density of an "effective" medium containing both the parent material and the evolving microstructure (e.g. vacancies, dislocations and other structural defects carrying the plastic strain). By further assuming that the effective mass density is proportional to the density of the carriers of plastic deformation γ, one can re-write Eq. (24) in the form

$$\dot{\gamma} + \mathrm{div}\,\mathbf{q} = \hat{g}, \tag{25}$$

where $\dot{\gamma}$ denotes the rate of plastic strain, $\mathbf{q}$ is the flux of plastic strain through the elementary representative volume and $\hat{g}$ is a source/sink term. While, in general, $\hat{g}$ may include both nucleation/annihilation of defects within the elementary representative volume along with losses/production on the surface, in the case of nanopolycrystals this term is dominated by grain boundary and other internal surface (triple grain boundary junction) processes.

It is pointed out that Eq. (25) may be viewed as a "complete balance law" for the internal variables containing both a flux and a source term (Aifantis, 1978). In this case where $\dot{\gamma}$ appears as a field variable in the governing equations, the effective stress τ and effective strain γ should generally be considered as independent variables so that $\hat{g} = g(\tau, \gamma)$. Furthermore, by assuming that the flux $\mathbf{q}$ is of a diffusive nature, say $\mathbf{q} = -D_\gamma \nabla\gamma + D_\tau \nabla\tau$, the following equation may be derived for the evolution of the equivalent plastic strain γ

$$\dot{\gamma} = g(\tau, \gamma) + D_\gamma \nabla^2 \gamma - D_\tau \nabla^2 \tau. \tag{26}$$

The one-dimensional form of Eq. (26) for tensile deformation with $D_\tau = 0$ and $g(\sigma, \varepsilon) = \dot{\varepsilon}_0 \sinh[\{\sigma - \sigma_L - h(\varepsilon)\}/s]$; $h(\varepsilon) = -h_0\varepsilon[1 - (\varepsilon/\varepsilon_L)^n]$ may be used to model (Aifantis, 1992) the propagation of Lüders bands (ε_L, σ_L, $\dot{\varepsilon}_0$, h_0, s, n are all constants with ε_L and σ_L denoting Lüders strain and stress respectively).

4. Three key basic problems

In this section we consider three basic key problems for gradient elasticity and gradient plasticity. The first is concerned with the elimination of stress/strain singularities from a mode-I micro/nano crack tip within the structure of the robust version of gradient elasticity, and the second problem with the modification of Johnson's spherical cavity model during micro/nano indentation within a robust gradient plasticity framework. The third problem is concerned with strain band nucleation and propagation within a simple gradient plasticity framework where, in addition to deterministic gradients, random effects in the flow stress expression are also introduced.

4.1. Elimination of singularities at the tips of nanocracks

As discussed earlier, the stress tensor σ_{ij} for a loaded nc or ufg material weakened by a (nano) crack, is given by the inhomogeneous Helmholtz equation (Aifantis, 2003, 2009a, 2009b) $\sigma_{ij} - c\nabla^2\sigma_{ij} = \sigma^0_{ij}$, where σ^0_{ij} is the classical elasticity solution with the well-known $r^{-1/2}$ singularity. For example, the σ_{22} component is determined from the differential equation

$$\sigma_{22} - c\nabla^2\sigma_{22} = \frac{K_I}{\sqrt{2\pi r}}\left[\cos\frac{\theta}{2}\left(1 + \sin\frac{\theta}{2}\sin\frac{3\theta}{2}\right)\right], \tag{27}$$

where $K_{\mathrm{I}} = \sigma^\infty\sqrt{\pi a}$ is the usual stress intensity factor for mode I (σ^∞ is the applied tensile stress at infinity and a is the half crack length), and (r, θ) are the usual polar coordinates with origin at the crack tip. By writing the angular component in Eq. (27) as [(5/4) cos θ/2 – (1/4)cos 5θ/2], splitting the deduced equation in two parts, solving the two resulting inhomogeneous Helmholtz equations separately by using superposition and, finally, taking into account the boundary conditions $\sigma_{ij} \to \sigma^0_{ij}$ as $r \to \infty$ and $r \to 0$, it turns out that under certain conditions the relevant non-singular asymptotic solution can be cast in the form

$$\sigma_{22} = \frac{K_{\mathrm{I}}}{\sqrt{2\pi r}}\left[\cos\frac{\theta}{2}\left(1 + \sin\frac{\theta}{2}\sin\frac{3\theta}{2}\right)\right](1 - e^{-r/\sqrt{c}}), \tag{28}$$

the distribution of which is given in Fig. 1 where scaled quantities $a^* = a/\sqrt{c}$ and $r^* = r/\sqrt{c}$ have been used in the plots. Non-asymptotic results and more complete expressions for all components of stress and strain, along with gradient-dependent fracture criteria, are postponed until a future publication.

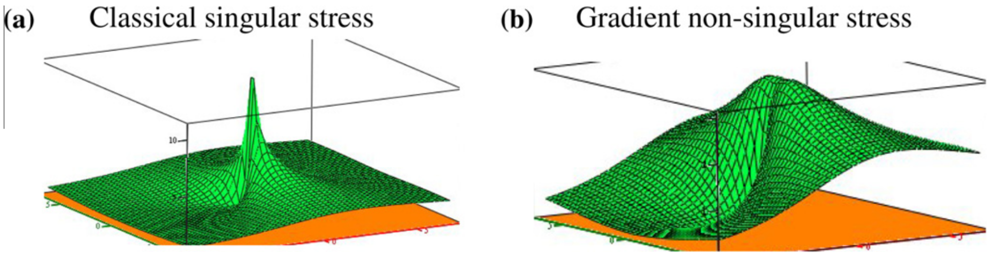

Fig. 1. Distribution of σ_{22} at the crack tip: (a) Classical singular stress; (b) Gradient non-singular stress.

Alternative forms for the mode I solution can be obtained if different boundary conditions along the crack surface are adopted. One such solution turns out to be composed from the usual elastic part and an additional term which varies as $r^{-3/2}$, thus recovering the form obtained by others [see, for example, Georgiadis, 2003; Karlis et al., 2007; Stamoulis & Giannakopoulos, 2008 and references quoted in Aifantis (2009b)], which in this author's opinion does not repair the weaknesses of classical fracture mechanics. A detailed discussion on the various forms of solutions at the crack tip (singular or not) and their relevance to nc and ufg materials should be conducted in relation to possible experiments carried out for such configurations.

4.2. Revisit of Johnson's spherical cavity model

Johnson's spherical cavity model for indentation was revisited in Mokios and Aifantis (2007) within a deformation version of gradient plasticity theory of Eq. (19). The schematics for this model are shown in Fig. 2a. On adopting Johnson's (1985) geometric similarity $\{\mathrm{d}a/\mathrm{d}r_{ep} = a/r_{ep}\}$ and hydrostatic core incompressibility $\{\pi a^2\,\mathrm{d}h = \pi a^2(\tan\beta)\mathrm{d}a = 2\pi r_{ep}^2[\partial u_r(r_{ep})/\partial r_{ep}]\mathrm{d}r_{ep}\}$ conditions, along with a perfect plasticity gradient yield condition $\bar{\sigma} = \sigma_Y - c\nabla^2\bar{\varepsilon}$ $(\bar{\sigma} = \sqrt{3/2\sigma'_{ij}\sigma'_{ij}};\ \bar{\varepsilon} = \sqrt{2/3\varepsilon'_{ij}\varepsilon'_{ij}})$, the spherical cavity model is solved again and modified expressions of the radial displacement $u(r)$ and the traction $t(r)$ are derived, namely

$$\begin{aligned} &u(r) = (r_{ep}^3/r^2)(\sigma_Y(1+\nu)/3E)[r_{ep}^2/(r_{ep}^2+4\ell^2)]; \quad \ell^2 \equiv c/(1+\nu)E, \\ &t(r) = -(2\sigma_Y/3) - 2\sigma_Y\log(r_{ep}/r) - [\{4\sigma_Y\ell^2/15(r_{ep}^2+4\ell^2)\}\{9(r_{ep}/r)^5 - 19\}], \end{aligned} \tag{29}$$

where (ν, E) denote elastic moduli, σ_Y is the yield stress, and the rest of the quantities are depicted in the sketch of Fig. 2a; the terms in the brackets of Eq. (29) are the corrections to the classical expressions due to the inclusion of gradients measured by the internal length ℓ. Then, the graph in Fig. 2b and its comparison with the experiment (McElhaney, Vlassak, & Nix, 1998) is obtained by assuming that the ratio of the hardness H over the yield stress σ_Y is proportional to the ratio of p_{int}/σ_Y. [The internal pressure p_{int} at $r = a$ equals to $-t(a)$ as imposed by the corresponding boundary condition.]

4.3. Front propagation

In this section the problem of neck or shear band front propagation is considered by incorporating random effects in the deterministic one-dimensional stress–strain gradient constitutive equation $\sigma = \kappa(\varepsilon) - c(\partial^2\varepsilon/\partial x^2)$. This, in view of the

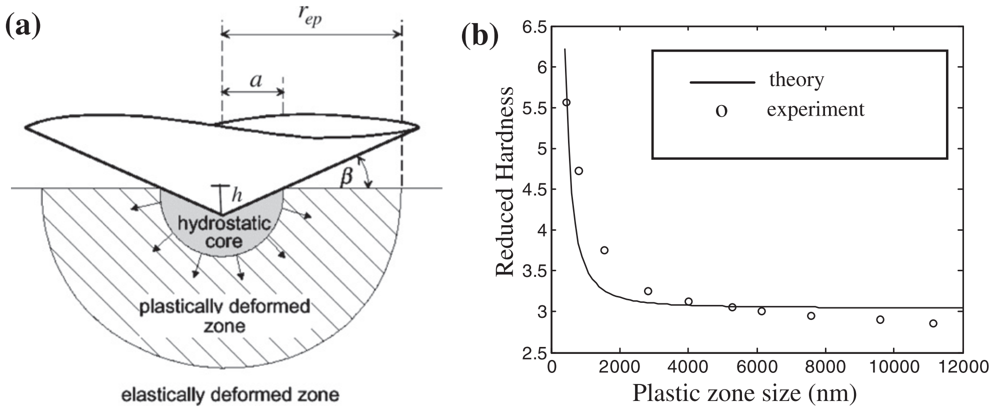

Fig. 2. (a) Schematics of Johnson's spherical cavity model; (b) Comparison with experiment (E = 130 GPa; ν = 0.34; σ_Y = 0.36 GPa; ℓ = 13.5 nm).

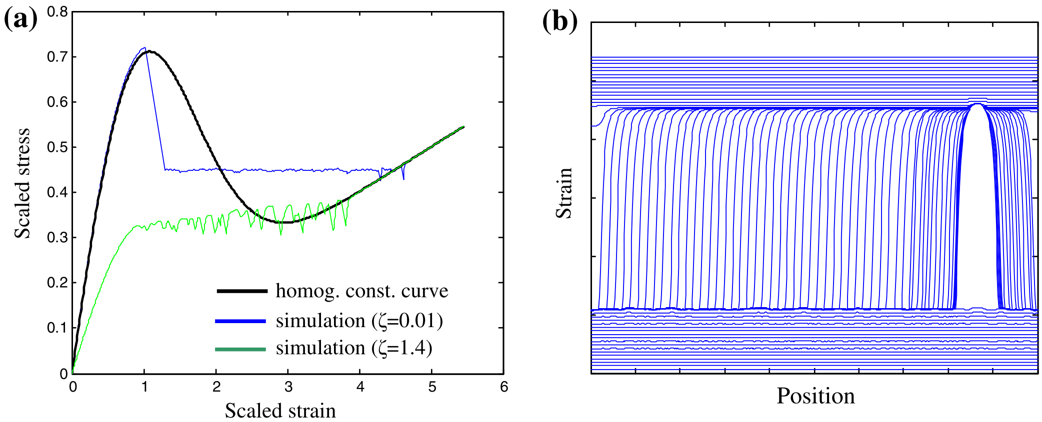

Fig. 3. (a) Stress–strain graphs showing the homogeneous constitutive curve (black) as well as a simulation curves obtained for low (blue) and high (green) randomness; (b) Strain distribution plots at various instances during the simulation (for $\zeta = 0.01$) showing the formation and propagation of localization bands. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article; the same should be done for the colored graphs in Fig. 4).

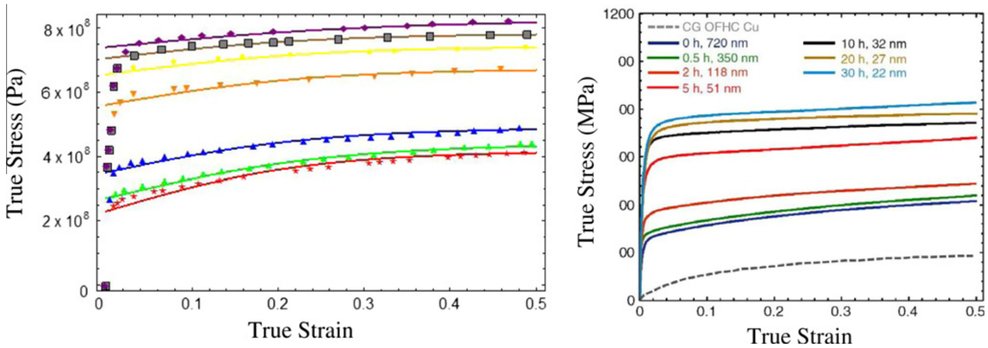

Fig. 4. Comparison between theory and experiment for nc-Cu samples of varying grain size.

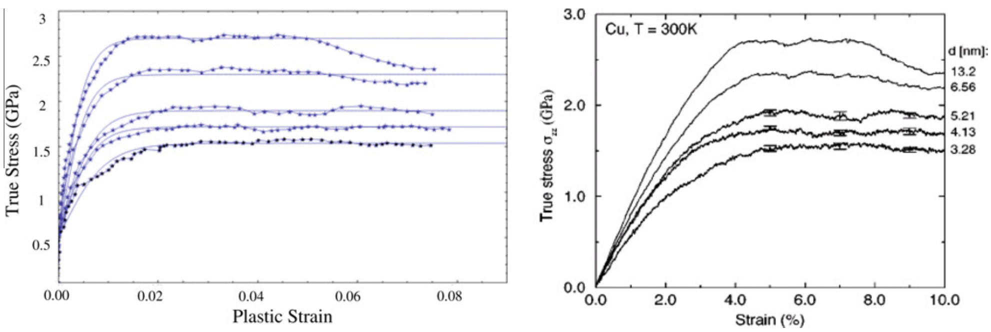

Fig. 5. Comparison between theory and simulations for nc-Cu sample of varying grain size.

one-dimensional equilibrium equation $\partial\sigma/\partial x = 0$, results to the governing differential equation $\sigma_0 = \kappa(\varepsilon) - c(\partial^2\varepsilon/\partial x^2)$, where x denotes the direction of front propagation. By introducing small perturbations $(\delta\varepsilon, \delta\sigma)$ due to disorder or random effects in the strain $(\varepsilon \to \varepsilon + \delta\varepsilon)$ and stress $(\sigma \to \sigma + \delta\sigma)$ fields (leading to a fluctuating flow stress $\kappa(\varepsilon) \to \kappa(\varepsilon) + \zeta k(\varepsilon, x)$, where ζ is a "small" parameter), we have $\sigma_0 = \kappa(\varepsilon) + \zeta k(\varepsilon, x) - c(\partial^2\varepsilon/\partial x^2)$; this being the governing equation defining the evolution of the strain front in the presence of both deterministic gradients and stochasticity.

To proceed further, we consider the following form for the random contribution $k(\varepsilon, x)$ to the flow stress expression: $k(\varepsilon, x) = f(\varepsilon)g(x)$; i.e. we assume separable contributions of the strain and the space field. We consider, in addition, short-range correlations in space, such that the autocorrelation of $g(x)$ is given by $\langle g(x)g(x')\rangle = \xi\delta(x - x')$, where $\xi = \ell_{corr}$ is the correlation length and $\delta(x-x')$ denotes the usual delta function. It follows that the variance of the stress perturbations is given by $\langle\delta\sigma^2\rangle=\xi[\zeta^2/(\Delta\varepsilon_f)^2]\int_{-\infty}^{\infty}f^2(\varepsilon)\varepsilon_{,x}\,dx$, where $\Delta\varepsilon_f=\varepsilon(-\infty)$ denotes the strain at infinity.

By choosing $f(\varepsilon)=\varepsilon e^{-\varepsilon^2/2}$ and $\kappa(\varepsilon)=\varepsilon e^{-\varepsilon^2/2}+h\varepsilon$ (h denotes linear hardening) one can calculate explicitly the variance $\langle\delta\sigma^2\rangle=\xi(\zeta/\Delta\varepsilon_f)^2\int_{\varepsilon_{-\infty}}^{\varepsilon_\infty}\{-2[e^{-\varepsilon^2/2}-(h/2)\varepsilon^2+\sigma_0\varepsilon-V(\varepsilon_\infty)]\}\varepsilon^2e^{-\varepsilon^2}\,d\varepsilon$, where $V(\varepsilon)=e^{-\varepsilon^2/2}-(h/2)\varepsilon^2$. By employing then a cellular automaton numerical scheme, one can obtain the graphs of Fig. 3. These preliminary results will be thoroughly discussed in a future publication considering the effect of the competition between deterministic strain gradients and randomness on the occurrence and evolution of plastic instabilities (Zaiser & Aifantis, 2003, 2006).

5. Stress–strain relations for nanopolycrystals

The reason for including this final section is to support the view that such type of gradient or nonlocal dependence in standard constitutive equations may provide a quick and easy-to-use tool for capturing mechanical behavior at the nanoscale. At the nanoscale, the representative elementary volume (REV) assumed for a continuum mechanics treatment is highly heterogeneous and may not be sufficiently described by local fields as is the case at the macroscale, where the corresponding heterogeneity can be “smoothed out” for stable deformations. In a first approximation then, the introduction of spatial gradients in the constitutive equations offers an interesting robust approach for modeling nanostructures, size and surface effects in real time, as opposed to molecular dynamics simulations which are commonly used for modeling such effects but for unreasonably short times (or unrealistically very high strain rates).

A mixture rule argument has been used recently (Aifantis & Konstantinidis, 2009) to model full stress–stain graphs for nc metals with varying grain size. This modeling effort was based on a Voce’s type constitutive relation for the flow stress along with a Hall–Petch (H–P) dependence on the grain size within a gradient plasticity framework with interfacial energy (Aifantis & Willis, 2005). It turns out, however, that a simpler and rather intuitive procedure may also be adopted for this purpose. This procedure is based on the use of an approximate microscopic dimensionless argument to replace the gradient dependence of the flow stress on the grain size leading to H–P or inverse H–P relations for this quantity (as well as for the corresponding hardening modulus), depending on whether hardening or softening takes place in the grain boundary space.

Roughly speaking, a H–P relationship within the earlier discussed gradient plasticity framework – for example Eq. (12) with $c=c^*=\bar{c}^*=0$ – may be deduced as follows. For tensile loading within the aforementioned model, the yield stress may be written as $\sigma=\sigma_0+k\ell^{1/2}|\nabla\varepsilon|^{1/2}$, where k is a stress-like parameter and l is an internal length associated with dislocation spacing or dislocation source distance. [Strictly speaking, such relation is deduced by slightly generalizing the dependence on $\nabla\gamma.\nabla\gamma$ in Eq. (12) to read $(\nabla\gamma.\nabla\gamma)^{m}$ and taking $m=1/4$. This choice of m can be justified on physical grounds by assuming a Taylor expression for the flow stress where, however, the effect of statistically and geometrically necessary dislocations is additively considered.] For a grain size d, the gradient term $|\nabla\varepsilon|^{1/2}$ may be approximated as $(\epsilon_0/d)^{1/2}$ with ϵ_0 denoting a reference strain. This yields a H–P relation for σ when the grain boundary hardens and an inverse H–P relation when the grain boundary softens. A similar argument can lead to analogous H–P dependencies for the hardening modulus h.

Next, we assume that the flow stress is given by the Voce-type relation

$$\sigma=\sigma_f+(\sigma_s-\sigma_f)\tanh[h\varepsilon/(\sigma_s-\sigma_f)], \tag{30}$$

where $\sigma_{s,f}=\sigma^o_{s,f}+k_{s,f}d^{-1/2}$ denote saturation and friction stresses respectively, and $h=h_0-k_hd^{-1/2}$ is a hardening like modulus. Then, one may obtain the model predictions depicted in Fig. 4a (solid lines) and their comparison with experimental data (Khan, Farrokh, & Takacs, 2008) as detailed in Fig. 4b. The parameter values used are $\sigma^0_s=230$ MPa, $k_s=92.5$ kPa $\sqrt{\text{m}}$; $\sigma^0_f=70$ MPa, $k_f=104$ kPa $\sqrt{\text{m}}$, $h_0=827$ MPa, $k_h=86$ kPa $\sqrt{\text{m}}$.

The same expression for the flow stress, i.e. Eq. (30), can be used for modeling simulation results for smaller grain sizes where an inverse H–P behavior has been documented (Schiøtz, Vegge, di Tolla, & Jacobsen, 1999) as shown in Fig. 5.

The parameter values used for the fits of Fig. 5a are $\sigma_f=500$ MPa; $\sigma_s=\sigma^0_s-k_sd^{-1/2}$, $\sigma^0_s=3920$ MPa, $k_s=140$ kPa $\sqrt{\text{m}}$; $h=h_0-k_hd^{-1/2}$, $h_0=730$ GPa, $k_h=34$ MPa $\sqrt{\text{m}}$. More details on such type of modeling and comparison with experiments will be reported by K.E. Aifantis and co-workers (Zhang, Romanov, & Aifantis, 2011).

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