

GRADIENT EFFECTS AT MACRO, MICRO, AND NANO SCALES

Elias C. Aifantis
Center for Mechanics of Materials and Instabilities,
Michigan Technological University, Houghton, MI 49931, USA
Laboratory of Mechanics
Aristotle University of Thessaloniki, Thessaloniki 540 06, GREECE

ABSTRACT

The effects of gradients on the localization and patterning of deformation at various scales ranging from the millimeter (macroscale) down to the nanometer (nanoscale) are discussed. At the nanoscale, a dominant mechanism of deformation is the rearrangement of free nano volume and exchange of momentum between bulk and grain boundary space. At the microscale, a most common mechanism of deformation is dislocation motion. At the macroscale, deformation patterning occurs by the transport of strain from one region of the deforming material to another. In each case, higher order gradients of the respective nano, micro or macro variables are essential to be included in the constitutive equations. This leads to various classes of material behavior including a gradient theory of elasticity, a gradient theory of defect dynamics, and a gradient theory of macroscopic plasticity. Within such "internal-length" theories it is possible to discuss the occurrence of deformation patterns at various scales, the determination of width, spacing and velocity of deformation bands, as well as the structure of the crack tip and the removal of associated strain or stress singularities.

1. INTRODUCTION

One of the outstanding problems in the mechanical behavior of materials has been the connection between micro ($\sim 10 - 100 \mu\text{m}$) and macro ($\sim 0.1 - 1.00 \text{ mm}$ or larger) scales. Recently, substantial attention has been given to materials at the nanometer scale ($\sim 10 - 100 \text{ nm}$ grain size) with the question of interest here being the determination of the coupling between nano and micro scales and its effect on the overall macroscopic response. The first step in addressing this question is to elucidate the mechanisms of deformation at various scales for all three regimes: prelocalization, postlocalization and fracture.

At the nanoscale, recent arguments suggest that elastic deformation may not be described by the standard theory of elasticity, but surface-tension like effects should be included through the incorporation of higher order gradients in the stress-strain relation. Plastic deformation occurs via the rearrangement and production of free volume associated with nanopores at

triple grain boundary junctions, while dislocation activity is usually confined within the grain boundary space only. Moreover, grain "stretching", "rotation" and "sliding", as well as "nano damage" development has been observed. At the microscale, the usual deformation mechanism is dislocation motion and production within the grains, while grain boundaries may act as obstacles or sources to dislocation motion or production. Again, "micro damage" formation is another mechanism of irreversible deformation, either independent or indirectly related to dislocation activity. Effectively, these mechanisms may be responsible for the development of high strain or stress gradients at the macroscale and the transport of strain from one material region to another. It turns out that these mechanisms of nano-, micro-, or macro-strain transport may act, indeed, as stabilizing mechanisms when the local homogeneous material response loses stability as a result of the external load exceeding a certain threshold. In fact, the most common way that a material responds to an increasing external stress before fracture, is to undergo through the occurrence of a "continuous" hierarchy of pattern-forming instabilities ranging from single dislocations and dislocation pileups to complex dislocation structures, shear bands and cracks.

A general framework for connecting micro to macro scales based on the concept of "normal" and "excited" states has been proposed by the author and his co-workers in the last decade. Within this program, "standard" and "non-standard" models of macroscopic plasticity were obtained on the basis of crystal slip and dislocation motion, and a justification for introducing higher order gradients of strain into corresponding constitutive equations was provided. These physically based non-standard plasticity models have led to a direct interpretation of axial effects in torsion. The higher order gradients have led to a direct interpretation of measurements pertaining to shear bands widths and spacings. The notion of normal and excited states may also be extended to describe deformation mechanisms occurring at the nanoscale. Nanostructural materials exhibit a large surface-to-volume ratio and, as a result, the material element may be viewed as a superposition of "surface" and "bulk" continua with each one supporting its own mechanical (stress and strain) fields. Moreover, they are allowed to exchange effective mass and momentum with each other in a manner consistent with the overall mass and momentum balance of the two superimposed continua considered as a whole. In fact, it can be shown that if (for moderate stress levels) both the bulk and grain boundary phases deform elastically and the interaction force is proportional to the relative displacement, then the governing differential equation is equivalent to that obtained from a direct second order strain gradient extension of Hooke's law. The corresponding second order stress is a surface tension-like stress similar in nature to the capillary force in the theory of inhomogeneous fluids.

In this paper, gradient effects on deformation processes occurring at the nano, micro, and macro scale are discussed. It is shown that higher order gradients are essential in capturing the heterogeneity of deformation and associated pattern-forming instabilities. At the nanoscale, the implications of a gradient theory of elasticity on the structure of the crack tip and the elimination of associated singularities are discussed. Moreover, a preliminary discussion of gradient effects on plastic flow and damage development at the nanoscale and some remarks on the "inverse" flow stress-grain size dependence observed in nanocrystalline materials are given. At the microscale (or mesoscale), gradient effects are accounted for through higher order gradients in defect (e.g. dislocations) densities modelling the relevant short-range interactions, with the corresponding long-range

interactions being screened due to the relatively high densities of defects or clusters of defects usually present in the cases under consideration. It is shown that these gradients are essential in modelling the self-organization of defects and dislocation patterning phenomena occurring at the micro (or meso) scale. The resultant theoretical framework may be termed dislocation-gradient dynamics. Finally, at the macroscale, gradient effects are most conveniently incorporated into the yield condition or the evolution equation for the back stress with the rest of the equations being the same as in the classical theory of plasticity. It has already been shown by the author and his co-workers that such a gradient dependence provides an appropriate internal-length scale to the structure of classical theory of plasticity, thus allowing the derivation of shear band widths and spacings in the post-instability regime. As this question has been addressed elsewhere for isothermal conditions, attention is confined here in illustrating the role of higher order gradients on the problem of thermoplastic instability with emphasis on the coupling between nonlinearity, strain gradients, and temperature gradients. Moreover, it is shown how a previous difficulty encountered in analyses pertaining to the velocity determination of Portevin Le Chatelier (PLC) bands is removed.

The various ideas are presented in the order that they were developed chronologically. Thus, microscales (or mesoscales) are considered first by modelling the gradient-dependent evolution of defects and the corresponding dislocation patterns. Then, macroscales are discussed by modelling gradient-dependent thermoplastic flow phenomena with reference to adiabatic shear banding. Finally, the nanoscale is addressed by modelling elastic nano deformation via a gradient-dependent elasticity theory (describing, among other things, surface-dependent deformation phenomena such as those occurring at crack tips) and plastic nano deformation via a gradient-dependent plasticity theory (describing, among other things, the evolution and transport of nano pores and nano damage development). To facilitate the discussion, however, a brief account motivating the need of higher order gradients for each class of the aforementioned deformation problems is given in the next section. In fact, the material of the next section (Section 2), as well as that of the subsequent section (Section 3), borrows heavily from a recent lecture of the author. [Keynote Lecture at the 7th Int. Symp. on Continuum Models of Discrete Systems, Paderborn, Germany June 14-19, 1992. Proceedings to be published by Trans Tech, eds. K.-H. Anthony and H.-J. Wagner, Materials Science Forum, Volumes 123-125, 1993.]

2. MOTIVATION FOR HIGHER ORDER GRADIENTS

The ultimate problem in continuum mechanics is the determination of stress and strain fields $\underline{\sigma}$ and $\underline{\epsilon}$ from the differential equations of dynamic equilibrium (or the local statements of conservation of linear and angular momenta),

$$\text{div } \underline{\sigma} = \rho \underline{\ddot{u}}; \quad \underline{\sigma} = \underline{\sigma}^T, \quad (2.1)$$

the stress-strain or constitutive relation

$$\underline{\sigma} = \underline{f}(\underline{\epsilon}), \quad (2.2)$$

and the strain-displacement relation, which for small deformations, reads

$$\underline{\underline{\epsilon}} = \frac{1}{2} (\nabla \underline{\underline{u}} + \nabla \underline{\underline{u}}^T) . \quad (2.3)$$

The symbols div and ∇ denote the divergence and gradient operators respectively, a superimposed dot denotes material time differentiation, a superimposed T denotes transpose, ρ is the mass density, $\underline{\underline{u}}$ is the displacement and the quantity $\underline{\underline{f}}$ is a tensor function of the present value (elasticity) or the history (viscoelasticity) of the strain $\underline{\underline{\epsilon}}$. In some models of generalized continua, such as Cosserat or multipolar media, the stress tensor may not be symmetric ($\underline{\underline{\sigma}} \neq \underline{\underline{\sigma}}^T$).

An excessively large number of variants of equation (2.2) has been proposed in the past to such a degree that a special research area commonly known as "constitutive theory" has been developed. Thus, the quantity $\underline{\underline{f}}$ could be a linear or nonlinear (convex or nonconvex) function of strain $\underline{\underline{\epsilon}}$. It may also depend on first or higher order time derivatives of $\underline{\underline{\epsilon}}$ or an additional set of (scalar, vector or tensor) internal variables $\underline{\underline{\alpha}}$ modelling the evolution of microstructure.

Such models of constitutive behavior for solid materials are not suitable for capturing the occurrence of pattern-forming instabilities. This is due to the fact that they do not possess an internal length to provide the governing differential equations with sufficient structure for analyzing the evolution of deformation in the post-instability regime. In this connection, it is emphasized that certain higher order continua such as Cosserat, multipolar or nonlocal media are usually characterized by a complex inhomogeneous spatial structure which, in principle, is amenable to instability analysis. However, the homogeneous part of the corresponding stress-strain relation was assumed to be either linear or convex nonlinear (strain hardening regime). Thus, these models could only predict stable homogeneous or nearly homogeneous deformation states and were not suitable for the analysis of deformation patterns.

To make this point more clear, we list below the constitutive equations for the following four typical classes of deformation behavior:

(i) Linear Elasticity:

$$\underline{\underline{\sigma}} = \lambda(\text{tr} \underline{\underline{\epsilon}}) \underline{\underline{1}} + 2\mu \underline{\underline{\epsilon}} , \quad (2.4)$$

where λ and μ are the Lamé constants.

(ii) Rigid Plasticity:

$$\underline{\underline{\sigma}} = -p \underline{\underline{1}} + 2\mu \dot{\underline{\underline{\epsilon}}} ; \quad \text{tr} \dot{\underline{\underline{\epsilon}}} = 0 ; \quad \tau = \kappa(\gamma) , \quad (2.5)$$

where the viscosity-like coefficient μ is now given by the ratio $\mu = \tau / \dot{\gamma}$ with $\tau = \sqrt{\frac{1}{2} \underline{\underline{\sigma}}' \cdot \underline{\underline{\sigma}}'}$ being the shear stress intensity or equivalent stress and γ

being the shear strain intensity or equivalent strain $\gamma = \int \dot{\gamma} dt = \int \sqrt{2 \dot{\underline{\epsilon}} \cdot \dot{\underline{\epsilon}}} dt$, while a dot and a prime denote inner product and deviatoric part respectively. The quantity p in the stress-strain relation (2.5)₁ is the hydrostatic pressure, equation (2.5)₂ is a statement of incompressibility, while equation (2.5)₃ expresses the yield condition.

(iii) Internal Variables:

$$\underline{\sigma} = \underline{f}(\underline{\epsilon}, \underline{\alpha}) \quad , \quad \dot{\underline{\alpha}} = \underline{g}(\underline{\epsilon}, \underline{\alpha}) \quad , \quad (2.6)$$

where $\underline{f}$ and $\underline{g}$ are functions whose structure is motivated by microscopic theory and experiment and $\underline{\alpha}$ is a measure of the internal state of the material. It can be related to dislocation density in a metal, to molecular chain configuration in a polymer, or to void concentration in a porous rock. It is worth noting that equation (2.6)₂, i.e. the evolution equation for the internal variables, includes only the generation or source term $\underline{g}$ of the relevant microstructures within an elementary material volume, but it neglects the transport or flux of microstructures through the boundaries of this material element. Complete balance laws for the internal variables containing both a rate and a flux or divergence term have been suggested by the author in the past and specific forms will also be discussed below.

(iv) Dislocation Kinetics:

$$\dot{\rho}_N = g(\rho_N, \underline{\sigma}, \dots) \quad ; \quad N = 1, 2, \dots, \quad (2.7)$$

where ρ_N denotes the density of the N^{th} family of dislocations and the dependence on the dislocation velocity is implicitly included through the dependence on $\underline{\sigma}$. Equations of the type (2.7) have been used excessively in the materials science literature for modelling plastic flow and they are commonly known as the equations of dislocation dynamics (in analogy to population dynamics in biology). Again, no flux or divergence terms are contained in equations (2.7) and, therefore, they are not suitable for predicting the routinely observed dislocation patterns. Divergence terms modelling the flux of dislocations within the elementary volume for certain simplified material geometries were first introduced in the papers of the author and his co-workers in order to model dislocation patterning phenomena and the corresponding framework was termed "gradient dislocation dynamics".

To contrast the above classes of constitutive equations with other model equations of physical and chemical systems which are amenable to pattern-forming instability analyses, we list below the Navier-Stokes equations of incompressible fluid mechanics, i.e.

$$-\nabla p + \mu \nabla^2 \underline{v} = \rho \left[\frac{\partial \underline{v}}{\partial t} + (\underline{\nabla} \underline{v}) \underline{v} \right] \quad , \quad (2.8)$$

and the Reaction-Diffusion equations for a system of interdiffusing and chemically interacting N species, i.e.

$$\dot{c}_i + D_i \nabla^2 c_i = g_i(c_j) ; (i, j) = 1, 2, \dots, N, \quad (2.9)$$

where p is the pressure, μ is the viscosity coefficient, ρ is the fluid density, c_i denotes concentration and D_i denotes diffusion coefficient.

Equation (2.8) is the result of substituting the constitutive equation for a viscous incompressible fluid $\underline{\sigma} = -p\mathbf{1} + \mu(\nabla \underline{v} + \nabla \underline{v}^T)$ into the momentum balance equation $\text{div} \underline{\sigma} = \rho \dot{\underline{v}}$. Equation (2.9) is the result of substituting the constitutive equation for the flux $\underline{j}_i$ of the i species $\underline{j}_i = -D_i \nabla c_i$ into the mass balance equation $\dot{c}_i + \text{div} \underline{j}_i = g_i(c_j)$, where the nonlinear source term g_i incorporates the effect of chemical reaction.

The rich pattern formation predicted by equations (2.8) or (2.9) is due to the competition of the gradient terms $\nabla^2 \underline{v}$ and nonlinear terms $(\nabla \underline{v}) \underline{v}$ in (2.8) or the gradient terms $\nabla^2 c_i$ and nonlinear terms $g_i(c_j)$ in (2.9).

This concludes our discussion concerning the motivation for incorporating higher order gradients in various model equations describing the spatio-temporal evolution of deformation at various scales of observation. Typical examples of such model equations for the deformation field at micro, macro and nano scales are given in the following sections.

3. MICROSCALES-GRADIENT DISLOCATION DYNAMICS

Higher order spatial gradients of dislocation densities were first introduced in the equations of dislocation dynamics in the papers of the author and his co-workers, [Aifantis (1984, 1985, 1986, 1987, 1988), Walgraef and Aifantis (1985, 1988, 1990)]. Various types of "gradient dislocation dynamics" were later adopted by several authors including Kubin and co-workers (1992), Kratochvil and co-workers (1992), Hahner (1992) and Romanov (1992) on the basis of physically motivated microscopic arguments. The original motivation for a "gradient dislocation dynamics" approach to plasticity was a balance equation for dislocation species of the form

$$\dot{\rho} + \text{div} \underline{j} = g, \quad (3.1)$$

with ρ denoting dislocation density, $\underline{j}$ denoting dislocation flux and g denoting dislocation production or annihilation.

As emphasized in Aifantis (1987), equation (3.1) is strictly valid for straight edge dislocations moving along their slip plane. The flux term $\text{div} \underline{j}$ is absent from usual Gilman-type dislocation dynamics equations, while the source term g is absent from the Kroner/Mura/Kosevich continuous distribution theory of moving dislocations. [As explained in Aifantis (1987), this theory proposes a balance law of the form $\dot{\underline{\alpha}} + \text{curl} \underline{J} = 0$ with $(\underline{\alpha}, \underline{J})$ designating the dislocation density and dislocation flux tensors respectively. In the case of a single family of straight edge dislocations the above tensor balance

equation reduces to the scalar balance equation (3.1) with the source term g set identically equal to zero]. Equation (3.1) may then be considered as a reasonable compromise between the approaches of dislocation dynamics and continuously distributed dislocations, especially in cases of high density of positive and negative dislocations, dislocation multipoles and dislocation walls routinely observed during monotonic or cyclic loading.

Equation (3.1) can be applied to various families and types of dislocations and other defects including positive and negative dislocations, mobile and immobile dislocations, as well as dislocation walls and declinations. The constitutive assumption usually employed for the flux $\underline{j}$ is such that a diffusive dislocation dynamics results from (3.1) and then a coupled system of reaction-diffusion like equations is obtained for the evolution of various defect populations.

As a representative example illustrating these ideas, we list the following set of general reaction-transport equations for dislocation species

$$\left. \begin{aligned} \dot{\rho}_i &= \nabla_i (D_{ij}^0 - D_{ijkl}^1 \nabla_k^2) \nabla_j \rho_i + g(\rho_i) - b\rho_i + \sum_n c_n \rho_i^n (\rho_m^+ + \rho_m^-), \\ \dot{\rho}_m^+ &= -v \nabla_x \rho_m^+ + \frac{b}{2} \rho_i - \sum_n c_n \rho_i^n \rho_m^+, \\ \dot{\rho}_m^- &= +v \nabla_x \rho_m^- + \frac{b}{2} \rho_i - \sum_n c_n \rho_i^n \rho_m^-. \end{aligned} \right\} \quad (3.2)$$

The indices (i, m) stand for immobile and mobile dislocations, while the superscripts $(+, -)$ stand for positive and negative dislocations. The terms $\pm v \nabla_x \rho_m^\pm$ result from the flux term $\text{div } \underline{j}_m$ on assuming that $\underline{j}_m = \rho_m^\pm \underline{v}^\pm \underline{e}_x$ and $\underline{v}^\pm = \pm v$, where $\underline{e}_x$ denotes the slip direction and ∇_x is the gradient in this direction. [The local dislocation velocity is assumed to be approximated by a spatially-independent average velocity v]. The terms $\sum_n \rho_i^n \rho_m$ represent interactions of mobile dislocations with immobile multipoles, while the tensors D_{ij}^0 and D_{ijkl}^1 are effective diffusion-like coefficients representing the anisotropic diffusive transport of immobile dislocations. Due to the attractive character of elastic interactions between dislocations, the tensor D_{ij}^0 may be negative definite in the high density regime, while D_{ijkl}^1 remains positive definite. By expressing the system of equations in terms of the sum $\rho_m = \rho_m^+ + \rho_m^-$ and the difference $\delta_m = \rho_m^+ - \rho_m^-$ we obtain

$$\left. \begin{aligned} \dot{\rho}_i &= \nabla_i (D_{ij}^0 - D_{ijkl}^1 \nabla_k^2) \nabla_j \rho_i + g(\rho_i) - b\rho_i + \sum_n c_n \rho_i^n \rho_m, \\ \dot{\rho}_m &= -v \nabla_x \delta_m + b\rho_i - \sum_n c_n \rho_i^n \rho_m, \\ \dot{\delta}_m &= -v \nabla_x \rho_m - \sum_n c_n \rho_i^n \delta_m. \end{aligned} \right\} \quad (3.3)$$

On assuming cyclic loading for which $v = v_0 \sin \omega t$ and for times scales larger than the period of the fatigue process, it turns out [e.g. Aifantis (1986)] that the "fast" variable δ_m can adiabatically be eliminated. Then equations (3.3)_{2,3} are replaced by a diffusion-like equation for the mobile

dislocations of the form

$$\dot{\rho}_m = D_m \nabla_x^2 \rho_m + b \rho_i - \sum_n c_n \rho_i^n \rho_m, \quad (3.4)$$

where the effective diffusivity D_m turns out to be given by the expression $D_m = v_o^2 / 2 \sum_n c_n \rho_{io}^n$ with ρ_{io} denoting a constant steady-state density. With this estimate for the effective diffusion coefficient of mobile dislocations and an analogous one for the diffusion coefficient $D_i = D_{xx}$ of the immobile dislocations of the form $D_i/a \approx \ell^2$, where ℓ is the annihilation distance of dipoles and $a = -g'(\rho_{io})$, we can predict the wavelength of the ladder structure of persistent slip bands for Cu single crystals in agreement with experiments. This prediction is readily obtained from the linear (Turing's type) instability analysis of the system of the reaction-diffusion equations (3.3)₁ and (3.4) giving a preferred wave number q_c

$$q_c = (a\gamma/D_i D_m)^{1/4}, \quad (3.5)$$

where $\gamma = \sum_n c_n \rho_{io}^n$. The spatially periodic structure is obtained when the bifurcation parameter b exceeds a critical value b_c^T , i.e.

$$b \geq b_c^T \equiv (\sqrt{a} + \sqrt{\gamma D_i/D_m})^2, \quad (3.6)$$

defining the onset of Turing's instability. A different threshold exists for a Hopf bifurcation of the form

$$b \geq b_c^H \equiv a + \gamma, \quad (3.7)$$

and this is associated with temporal dislocation oscillations which may effectively be related to the well-known Neumann's strain bursts. The above discussion holds for the later stages of deformation where the diffusion coefficient for the immobile dislocations is positive. At the initial stages, a diffusive instability may occur ($|D_{ij}^v| < 0$). It can then be shown that the above system of gradient dislocation dynamics can predict the appearance of cellular dislocation structures which can be identified with the so-called vein or matrix structure; [see, for example, the papers of Mughrabi quoted in Aifantis (1987)].

When a simplified version of the above reaction-diffusion approach to dislocation patterning was first presented, there was some concern with the physical basis of the diffusion-like terms for dislocation species, as well as with the specific form adopted for the nonlinear source term $\rho_i^n \rho_m$; [see, for example, the discussion by F.R.N. Nabarro in Aifantis (1986)]. Recent justification for the diffusive-like dynamics of dislocations has independently been provided by several authors including Kubin and co-workers (1992), Kratochvil and co-workers (1992), as well as Hahner (1992) and Romanov (1992) by adopting microscopic arguments based on cross slip, glide of

positive and negative dislocations, etc. The nonlinear $\rho_i^n \rho_m$ term was included to model interactions between immobile dislocation multipoles and mobile dislocations. Such higher order nonlinearities ($n \geq 2$), usually required for the stability of the resulting inhomogeneous periodic patterns, may also be formally obtained by assuming a lower order nonlinearity ($n = 1$) but also include the interaction with point defects in the form, say, $c_v \rho_i \rho_m$ where c_v denotes the concentration of point defects such as vacancies. The quantity c_v can then be adiabatically eliminated ($\dot{c}_v = 0$) through an evolution equation of the form, for example, $\dot{c}_v = A \rho_i c_v - B \rho_i^2$ (with A and B being rate constants). This gives a proportionality relation between c_v and ρ_i which upon substitution into the $\rho_i \rho_m$ term gives, in turn, the desired $\rho_i^2 \rho_m$ term.

An analogous adiabatic elimination argument can also be employed for generating higher order gradient terms in the usual equations of dislocation dynamics. This can readily be seen by considering a set of evolution equations of the form

$$\begin{aligned} \dot{\rho} &= g(\rho, c_\alpha) , \\ \dot{c}_\alpha &= D_\alpha \nabla^2 c_\alpha + r(c_\alpha, \rho) , \end{aligned} \quad (3.8)$$

where spatial gradients are not included in the evolution equation for the dislocation density ρ . Instead, the coupling with point defects c_α ($\alpha = i, v$) is included (c_i and c_v denote interstitial and vacancy concentration). Naturally, c_α obeys a diffusive dynamics which, in conjunction with the adiabatic elimination of c_α , gives an equation of the form

$$\dot{\rho} = g(\rho) + D \nabla^2 \rho - E \nabla^4 \rho + \dots, \quad (3.9)$$

where $g(\rho)$ is the "homogeneous" part of the source term $g(\rho, c_\alpha)$, while the gradient terms comprise the corresponding "inhomogeneous" part resulting from the adiabatic elimination of c_α ($\dot{c}_\alpha \sim 0$). For more details on such adiabatic elimination procedure one may consult a recent article by the author, Aifantis (1986), as well as a related short calculation given in the next section. A similar fourth order reaction-diffusion equation for dislocation species has recently been derived and analyzed by Franek et al (1981).

In concluding this section, we refer to preliminary work by Romanov and the author in modelling disclination-dislocation patterning phenomena by the reaction-diffusion scheme. Some model equations are reported in Romanov (1992) but a system which seems to be most promising for discussing the relevant effects is given by the equations

$$\begin{aligned} \dot{\rho} &= g(\rho) - b \rho^2 \varphi + D \nabla_{xx}^2 \rho , \\ \dot{\varphi} &= -r(\varphi) + d \rho^2 \varphi + D_p \nabla_p^2 \varphi , \end{aligned} \quad (3.10)$$

where φ denotes the density of disclinations and the rest of the quantities have their usual meaning.

4. MACROSCALES-GRADIENT PLASTICITY AND THERMOPLASTICITY

Higher order gradients have already been introduced into the macroscopic theory of plasticity by the author and his co-workers, as well as other investigators, in order to capture the thickness, spacing and velocity of shear bands. A most recent review of such a gradient approach to the heterogeneity of plastic flow can be found in a recent article by the author, Aifantis (1992). Here, it suffices to mention that the internal length scale is introduced to the aforementioned gradient-dependent theory of plasticity via a modification of the yield condition $\tau = \kappa(\gamma)$ (τ is the equivalent Mises stress and γ denotes the equivalent plastic strain) to include a term $c\nabla^2\gamma$ in its right hand side, where c is a gradient coefficient. A justification for such a type of gradient dependence of the flow stress can be obtained by allowing κ in the above relation to depend not only on γ but also on an internal variable α (e.g. point defect concentration) obeying a diffusive dynamics, say, of the form

$$\dot{\alpha} + D\nabla^2\alpha = g(\alpha, \gamma). \quad (4.1)$$

Then, the adiabatic elimination of α from the above equation and the flow condition $\tau = \kappa(\gamma, \alpha)$ yields the desired dependence of the flow stress on the second gradient of γ .

To see this explicitly, let us consider the corresponding one-dimensional problem in the form

$$\begin{aligned} \tau &= \kappa(\gamma, \alpha), \\ \dot{\alpha} &= D\partial_{xx}^2 \alpha + g(\gamma, \alpha), \end{aligned} \quad (4.2)$$

and adopt, for simplicity, a linear dependence of the hardening function $\kappa(\gamma, \alpha)$ on the internal variable α , as well as a linear dependence of the source function $g(\gamma, \alpha)$ on both γ and α . Thus, we have

$$\begin{aligned} \tau &= \hat{\kappa}(\gamma) - \lambda\alpha, \\ \dot{\alpha} &= D\alpha_{xx} + \Lambda\gamma - M\alpha, \end{aligned} \quad (4.3)$$

where α_{xx} denotes second partial derivative and (λ, Λ, M) are constants. The Fourier transform of (4.3)₂ gives

$$\dot{\alpha}_q = -Dq^2\alpha_q + \Lambda\gamma_q - M\alpha_q, \quad (4.4)$$

where q denotes the wave vector. The adiabatic elimination argument now suggests that α_q varies very rapidly in comparison to the other macroscopic variables of the system (i.e. the life-time of defects is much smaller than the corresponding time scales over which macroscopic variables evolve) and

therefore it can be eliminated ($\dot{\alpha}_q = 0$). It then follows from (4.4) that

$$\alpha_q = \frac{\Lambda}{M + Dq^2} \gamma_q, \quad (4.5)$$

which, by adopting a Taylor's series expansion for the term $\Lambda/(M + Dq^2)$ on the assumption that $(Dq^2/M) \ll 1$, gives

$$\alpha_q = \frac{\Lambda}{M} \gamma_q - \frac{\Lambda D}{M^2} q^2 \gamma_q, \quad (4.6)$$

or

$$\alpha = \frac{\Lambda}{M} \gamma + \frac{\Lambda D}{M^2} \gamma_{xx}. \quad (4.7)$$

Upon substitution of (4.7) into (4.3), we obtain a gradient-dependent yield condition of the form

$$\tau = \kappa(\gamma) - c\gamma_{xx}, \quad (4.8)$$

with $\kappa(\gamma) = \hat{\kappa}(\gamma) - (\lambda\Lambda/M)\gamma$ and $c \equiv \lambda(\Lambda D/M^2)$.

A quadratic nonlinear version of (4.8) which has successfully been used in the past, Aifantis (1984), reads

$$\tau = \kappa(\gamma) - c_1\gamma_{xx} - c_2\gamma_x^2, \quad (4.9)$$

and values for the gradient coefficients c_1 and c_2 have been inferred from shear band widths experiments, Zbib and Aifantis (1992). This was accomplished by substituting (4.9) into the corresponding one-dimensional equilibrium equation for the stress τ , i.e. $\partial\tau/\partial x = 0$, and then solving the resultant nonlinear differential equation under appropriate boundary conditions (i.e. $\gamma \rightarrow \gamma_0$ as $x \rightarrow \pm\infty$, $\gamma_x \rightarrow 0$ as $x \rightarrow \pm\infty$). The solution gives a bell-like profile for the strain γ and this, in turn, provides an estimate for the shear band thickness.

It is also interesting to study the situation in the case that τ in (4.9) does not evolve quasistatically ($\partial\tau/\partial x = 0$) but dynamically, such that

$$\frac{\partial\tau}{\partial x} = \rho_0 \ddot{u}, \quad (4.10)$$

with ρ_0 denoting a constant density and u the displacement ($\gamma = \partial u/\partial x$).

Substitution of (4.9) into (4.10) does not lead into an equation that can be solved analytically. Nevertheless, one can resort to stability analysis for understanding the basic behavior of the system. In fact, by assuming a homogeneous (but time-dependent) state (u_0, γ_0, τ_0) and perturbations $(\tilde{u}, \tilde{\gamma}, \tilde{\tau})$ such that $u = u_0 + \tilde{u}$, $\gamma = \gamma_0 + \tilde{\gamma}$, $\tau = \tau_0 + \tilde{\tau}$, it is possible to first ask

the question of whether the homogeneous state can become unstable in favor of infinitesimal periodic perturbations. If the answer to this question is affirmative, then one can ask a second question, i.e. whether the so-obtained periodic pattern persists (stable) or it evolves rapidly to another, possibly localized, one (unstable). The first question is addressed by employing standard linear stability analysis, while the second question can be addressed by employing the so-called Landau's or amplitude equations approach.

For convenience, a finite domain is assumed $0 \leq x \leq \pi$. The standard or "homogeneous" boundary conditions are taken, as usual, to be of the form $\tilde{u}(0, t) = 0$, $\tilde{u}(\pi, t) = u_0$, while the non-standard or "inhomogeneous" boundary conditions associated with the higher order gradient terms are assumed to be of the form $u_{xx}(0, t) = u_{xx}(\pi, t) = 0$.

For the linear stability analysis, the perturbation is assumed to be a modulation of the form

$$\tilde{u} = A(t) \sin qx, \quad A(t) = e^{i\omega t}, \quad (4.11)$$

where q denotes the wave number and $A(t)$ the corresponding amplitude, which evolves according to the standard exponential relation suggested by (4.11). The linear growth coefficient or eigenvalue ω and the critical or preferred wave number $q = q_c$ ($\omega = \omega_{\max} > 0$) are determined from the corresponding dispersion equation. This, in turn, is obtained by substituting (4.11) into the governing differential equations of the problem.

For the nonlinear stability analysis the amplitude $A(t)$ should first be defined from an equation, say, of the form

$$A(t) = \int_0^\pi \tilde{u}(x, t) \sin qx \, dx, \quad (4.12)$$

and then the expansions

$$\begin{aligned} \dot{A} &= \omega_1 A + \omega_2 A^2 + \omega_3 A^3, \\ \tilde{u} &= u_1(x)A + u_2(x)A^2 + u_3(x)A^3, \end{aligned} \quad (4.13)$$

are introduced into the governing differential equations to obtain appropriate expressions for the nonlinear growth coefficients $\omega_1 = \omega$, ω_2 and ω_3 . For the cases considered here it turns out that $\omega_2 = 0$ and thus the sign of ω_3 determines the nonlinear stability. In fact, when $\omega_3 > 0$ it follows that $A(t) \rightarrow \infty$ as $t \rightarrow \infty$ and the initially (linear) periodic pattern evolves "catastrophically" to a nonlinear, possibly periodic, one. In contrast, when $\omega_3 < 0$ it follows that $A(t) \rightarrow (-\omega_1/\omega_3)^{1/2}$ as $t \rightarrow \infty$ and the initially (linear) periodic pattern stabilizes to one with the same wavelength and an amplitude given as above. This type of "weakly nonlinear" analysis for deformation instability problems was adopted by Ru and Aifantis (1993) and the special results given in the remaining of this section are extracted from a preliminary

MM report as quoted in the list of references.

In the case that the flow stress $\tau = \kappa(\gamma)$ is expanded as

$$\kappa(\gamma) = \kappa(\gamma_0) + H\tilde{\gamma} + \frac{1}{2} F\tilde{\gamma}^2 + \frac{1}{6} G\tilde{\gamma}^3, \quad (4.14)$$

the linear stability analysis gives the following dispersion equation

$$-\omega^2 \rho_0 = (H + c_1 q^2) q^2. \quad (4.15)$$

It then follows that the critical point is $H = H_c = 0$ and that for the supercritical case $H < 0$ we find

$$\omega = \omega_c = \left(\frac{H^2}{4\rho_0 c_1} \right)^{1/2}; \quad q = q_c = \left(-\frac{H}{2c_1} \right)^{1/2}. \quad (4.16)$$

The importance of a non-vanishing c_1 in securing a finite linear growth ($\omega < \infty$) and a preferred wave number ($q = q_c$) is clearly seen. On the other hand, the nonlinear stability analysis, in the sense of (4.13), gives $\omega_2 = 0$ and

$$\omega_3 = \frac{H}{32\omega\rho_0 c_1^2} \left[\frac{2(2Hc_2 + Fc_1)(Hc_2 - Fc_1)}{3\pi^2 c_1^2} - \frac{GH}{\pi^2} \right]. \quad (4.17)$$

If the cubic nonlinearity is suppressed ($G = 0$), it follows that for $|c_1 F| \gg |c_2 H|$ we have

$$\omega_3 \approx -\frac{H F^2}{48\pi^2 \omega \rho_0 c_1^2} > 0, \quad (4.18)$$

while for $|c_1 F| \ll |c_2 H|$ we have

$$\omega_3 \approx -\frac{c_2^2 H^3}{24\pi^2 \omega \rho_0 c_1^4} < 0. \quad (4.19)$$

In the first case the initially periodic pattern becomes unstable, while in the second case (fulfilled, for example, when c_2 becomes important as compared to c_1) the initially periodic pattern stabilizes with an amplitude equal to $(-\omega/\omega_3)^{1/2}$. It is seen that the second gradient coefficient c_2 in (4.9) can

have a stabilizing effect on evolving strain modulations in softening materials.

For non-isothermal cases, equations (4.9) and (4.10) should be supplemented with the energy equation

$$\rho_o C \dot{\theta} = k \theta_{xx} + \beta \tau \dot{\gamma}, \quad (4.20)$$

where θ denotes temperature, C is the specific heat, k is the heat conductivity and β the Taylor-Quinney constant. Moreover, $\kappa(\gamma)$ in (4.9) depends on θ in a way such that $Q \equiv \partial \kappa(\gamma, \theta) / \partial \theta < 0$ (thermal softening). The hardening modulus is defined as before by $H = \partial \kappa(\gamma, \theta) / \partial \gamma$ and can be positive (strain hardening) or negative (strain softening). The appropriate boundary conditions are assumed to be of the form $\partial \theta / \partial x(0, t) = \partial \theta / \partial x(\pi, t) = 0$.

In the case of adiabatic shear, the conductivity may be taken as vanishingly small ($k = 0$), but $c_1 > 0$, and the corresponding critical condition reads

$$Q \beta \tau_o + H \rho_o C = 0, \quad (4.21)$$

indicating that it is independent of the gradient coefficient c_1 . For supercritical states $(Q \beta \tau_o + H \rho_o C) < 0$, H may be positive or negative, and the linear stability analysis gives

$$\omega = \frac{Q \beta \dot{\gamma}_o + (Q \beta^2 \dot{\gamma}_o^2 + 4 \rho_o C^2 c_1 q^4)^{1/2}}{2 \rho_o C} > 0, \quad (4.22)$$

$$q = q_c = \left(- \frac{Q \beta \tau_o + H \rho_o C}{2 \rho_o C c_1} \right)^{1/2}.$$

The non-vanishing of the gradient coefficient c_1 in securing a finite growth coefficient ω and a preferred wave number $q = q_c$ is clearly seen again. It turns out that a nonlinear thermoplastic analysis in the sense of (4.13), by adopting an expansion for $\bar{\theta}$ analogous to that of (4.13)₂, implies $\omega_2 = 0$ and $\omega_3 > 0$, i.e. the initial modulation evolves catastrophically to a different, possibly localized pattern.

In the case of non-vanishing conductivity ($k \neq 0$) but vanishing gradient coefficient ($c_1 \equiv 0$), it turns out that supercritical states ($\omega \geq 0$) require

$$(H \rho_o C + Q \beta \tau_o)^2 \geq - 4 Q H \rho_o \beta k \dot{\gamma}_o; \quad H \rho_o C + Q \beta \tau_o < 0, \quad (4.23)$$

and the corresponding dispersion equation gives

$$\omega = \frac{H\rho_o C - Q\beta\tau_o - 2 \left[-QH\rho_o \beta (C\tau_o + k\dot{\gamma}_o) \right]^{1/2}}{k\rho_o} , \quad (4.24)$$

$$q_c^4 = q^4 = \left(\frac{\rho_o^2 C \omega - \rho_o Q\beta\dot{\gamma}_o}{kH} \right) \omega^2 ,$$

implying that a preferred wave number is possible only when $H > 0$ (in contrast to the previous case of $c_1 \neq 0$, $k = 0$) where H could be positive or negative.

The nonlinear analysis, in this case implies as in the previous case $\omega_2 = 0$ and $\omega_3 > 0$.

As mentioned earlier, some of the results presented in the later portion of this section will be discussed in detail in a future article; see also the preliminary report by Ru and Aifantis (1993) quoted in the list of references. In this article, the case of vanishing inertia will also be considered by adopting a "weakly nonlinear" analysis approach. In this connection, it is pointed out that certain results based on a fully nonlinear analysis for the problem of thermoplastic instability has been given earlier by Charalambakis and Aifantis (1991). Moreover, a proposal for introducing higher order gradients of temperature in the energy equation was recently advanced by Aifantis (1992).

In concluding this section, it is pointed out that consideration of inertia through (4.10) and nonlinearity through (4.13) can remove some undesirable features of the marginal stability analysis employed by Zbib and Aifantis (1988) for determining the velocity of Portevin-Le Chatelier bands. The velocity selection problem for propagating plastic instabilities is addressed in a recent viewpoint set containing both theoretical and experimental contributions organized by Estrin et al and to be published in Scripta Met (1993). The gradient-dependent viscoplastic constitutive equation used by Zbib and Aifantis (see also Aifantis 1987) reads

$$\sigma = h\varepsilon + f(\dot{\varepsilon}) + c\varepsilon_{xx} , \quad (4.25)$$

with σ denoting the one-dimensional stress, ε being the corresponding strain, (h, c) denoting respectively the hardening and strain-gradient coefficients, and f being a non-convex function (single loop) of the strain rate $\dot{\varepsilon}$ with the negative slope portion ($f' < 0$) suggesting a negative strain rate sensitivity. By introducing (4.25) into the momentum equation

$$\partial_x \sigma = m\rho_o \partial_t^2 u , \quad (4.26)$$

with $m\rho_o$ denoting an effective mass density (m is an adjustable coefficient) and u being the displacement ($\varepsilon = \partial_x u$), we obtain from a linearized marginal stability-like analysis the following expression for the velocity $V = V^*$ of the propagating PLC bands

$$V^{*2} = \frac{h}{m\rho_o + [f'(z)/4c]} , \quad (4.27)$$

where $z = \dot{\epsilon}(x-Vt)$. It is seen that for $m\rho_0 \neq 0$ the previous (undesirable) divergence of the velocity V^* does not occur at the end points of the negative slope regime where $f' = 0$. Moreover, recent unpublished results by Ru and Aifantis (1993), based on a weakly nonlinear analysis for the perturbation at the leading edge, indicate that for the branch $f''(\dot{\epsilon}) < 0$, the velocity V_* is given by $V_*^2 = V^{*2}/2$ where V^* is the expression obtained from the linearized MSA given above. For the branch where $f''(\dot{\epsilon}) > 0$, the velocity is given by V^* . It thus follows that the above results, which originally seemed not to be in agreement (at least for the second branch $f'' > 0$) with the observations of Karimi on steel (suggesting that the velocity decreases with applied stress rate and vanishes at the upper end of the stress-strain rate graph) are not inconsistent with the experimental trends reported by McCormick et al in the viewpoint set mentioned above.

The state of affairs described above, especially the conflicting experimental results of Karimi and McCormick (see "Viewpoint Set on Propagative Plastic Instabilities" by Estrin et al, Scripta Meta, 1993), brings into a new perspective the analysis proposed by Jeanclaude et al (1992) for the PLC and it does not justifies some of their discussion and comments pertaining to the use of the constitutive equation (4.25) and the corresponding marginal stability analysis for determining the velocity of the PLC bands.

5. NANOSCALES-GRADIENT ELASTICITY AND MIXTURE APPROACH

A gradient theory of elasticity of the form

$$\underline{\sigma} = \lambda(\text{tr}\underline{\epsilon}) \underline{1} + 2\mu\underline{\epsilon} - c\nabla^2[\lambda(\text{tr}\underline{\epsilon})\underline{1} + 2\mu\underline{\epsilon}], \quad (5.1)$$

with c a constant has been proposed and utilized to eliminate the strain singularity in a Mode-III crack. [For an outline of the solution, the reader may again consult the previously mentioned review article of the author (Aifantis 1992)]. This theory is particularly suited for elastic deformations at the nanoscale, as well as for the description of the deformation field near elastic interfaces. It turns out, in particular, that if a nanophase material is assumed to consist of two superimposed states indicated by the indices 1 (for the bulk space) and 2 (for the grain boundary space), the equations of equilibrium read

$$\begin{aligned} \text{div } \underline{\sigma}_1 &= \underline{f}, \\ \text{div } \underline{\sigma}_2 &= -\underline{f}, \\ \text{div } \underline{\sigma} &= 0, \end{aligned} \quad (5.2)$$

where $\underline{\sigma} = \underline{\sigma}_1 + \underline{\sigma}_2$ is the total stress and $\underline{f}$ is an interaction force between the two phases. If both phases are deformed elastically, the following constitutive equations can be assumed

$$\left. \begin{aligned} \underline{\sigma}_k &= \underline{L}_k \underline{u}_k, \quad k = 1, 2; \quad \underline{f} = \alpha(\underline{u}_1 - \underline{u}_2), \\ \underline{L}_k &= \lambda_k \underline{G} + \mu_k \underline{\nabla}; \quad \underline{G} = \underline{1} \text{div}, \quad \underline{\nabla} = \underline{\nabla} + \underline{\nabla}^T. \end{aligned} \right\} \quad (5.3)$$

It follows that uncoupling of (5.2) and (5.3) results into the equation

$$\mu \nabla^2 \underline{u} + (\lambda + \mu) \nabla \operatorname{div} \underline{u} - c \nabla^2 [\mu \nabla^2 \underline{u} + (\lambda + \mu) \nabla \operatorname{div} \underline{u}] = 0, \quad (5.4)$$

if it is also assumed that the two superimposed phases have the same shear modulus; otherwise, two constants appear in the higher order gradient part of (5.4). It is apparent that (5.4) is the governing equation obtained by substituting the gradient elasticity constitutive equation (5.1) into the equilibrium equation (5.2).

It can be shown that for traction boundary conditions, solutions of equation (5.4) can be reduced to the classical elasticity solution in the following sense

$$\begin{aligned} \underline{\sigma} &= \underline{\sigma}^0, \\ (1 - c \nabla^2) \underline{u} &= \underline{u}^0; \quad \frac{\partial^2 \underline{u}}{\partial n^2} = 0. \end{aligned} \quad (5.5)$$

In equations (5.5), the superscript ⁰ denotes the classical elasticity solution and the boundary condition $\partial^2 \underline{u} / \partial n^2$ (with $\underline{n}$ denoting outward unit normal) is the extra boundary condition that also needs be assumed for the solution of the original problem (5.4). In fact, it turns out that within a "boundary layer approximation" for straight boundaries, condition (5.5)₂ is essentially implied by a variational argument.

By applying the above formulation to the solution of a straight crack, it turns out that due to (5.5)₁ the stress remains singular at the crack tip as in the classical theory, but the strain singularity is removed and the corresponding crack opening displacement (COD) $\delta = \delta(x)$ is obeying the differential equation

$$\delta - c \delta'' = \delta^0(x), \quad (5.6)$$

where $\delta^0(x) = b \sqrt{a^2 - x^2}$ is the classical elasticity COD with b denoting the (directional) stress-intensity factor and $2a$ denoting the crack length. If the boundary condition $\delta(\pm a) = 0$ is assumed, the solution of equation (5.6) is obtained as

$$\delta(x) = \frac{b}{\sqrt{c}} \left[\frac{\operatorname{sh}\left(\frac{\bar{a} + \bar{x}}{\sqrt{c}}\right)}{\operatorname{sh}\left(\frac{2a}{\sqrt{c}}\right)} \int_{-a}^{\bar{a}} \operatorname{sh}\left(\frac{a-s}{\sqrt{c}}\right) \sqrt{a^2 - s^2} ds - \int_{-a}^{\bar{x}} \operatorname{sh}\left(\frac{x-s}{\sqrt{c}}\right) \sqrt{a^2 - s^2} ds \right], \quad (5.7)$$

indicating that $\delta'(\pm a) \neq 0$, i.e. the strain is not singular at the crack tip. If the (boundary) condition $\partial^2 \underline{u} / \partial n^2 = 0$ is assumed everywhere along the crack axis ahead of the crack tip, an expression of the form $\underline{u} \sim e^{-x/\sqrt{c}}$ is obtained

for the displacement. This, in a (boundary layer) sense, establishes the "smooth crack closure" condition of Barenblatt. If a negative c is assumed, a "periodic" solution for the crack tip opening displacement (COD) is obtained. There is some evidence that periodic crack paths are possible prior to crack bifurcation. This is consistent with the present result since the condition $c < 0$ implies unstable behavior, as it can be concluded from a corresponding routine variational argument based on the strain energy density corresponding to constitutive equation (5.1).

The above framework can also be adopted for the analysis of an interface crack. It can be shown that the interpenetration condition is removed. This is because in contrast to the classical elasticity expression for the COD, i.e.

$$\delta_y^0 = b\sqrt{a^2 - x^2} \cos \gamma \theta, \quad \theta = \frac{1}{2} \log [(a+x)/(a-x)], \quad (5.8)$$

the present theory predicts the following expression for the derivative (strain) of δ_y at the crack tip

$$\delta_y'(-a) = \frac{b}{\cosh(\frac{2a}{c})} \int_{-a}^a \operatorname{sh} \left(\frac{a-s}{\sqrt{c}} \right) \sqrt{a^2 - s^2} \cos \left[\frac{\gamma}{2} \log \left(\frac{a+s}{a-s} \right) \right] ds, \quad (5.9)$$

which is a positive quantity. More details on the gradient elasticity and its implications can be found in the aforementioned preliminary report by Ru and Aifantis (1993).

In concluding the discussion on gradient elasticity effects at the nonoscale, it is pointed out that the constitutive equation (5.1) is not but a very special form of theory of elasticity with microstructure as proposed earlier by Toupin, Mindlin and others [for a list of references and related contributions see Kroner (1968)]. Moreover, the boundary conditions (5.5)₁ and (5.5)₃ turn out to be a special form of the more general boundary conditions derived from (5.1) and a variational argument similar to that earlier employed by Mindlin (1965) [see also Mindlin and Eshel (1968)]. In fact, the general boundary conditions reduce to (5.5)₁ and (5.5)₃ for straight boundaries such as those involved in crack problems ($y = \text{const.}$) under the "boundary layer-like" approximation that the variations in x are much smaller than the variations in y . Finally, it is pointed out that while the uniqueness of the solution of boundary value problems based on (5.1) requires a positive c , the wave propagation analysis suggests that c may be negative in order to obtain desirable dispersion results. In fact, the simplified dispersion analysis of harmonic waves based on a displacement field of the form

$$u(x, t) = u_0 \exp[i(qx - \omega t)], \quad (5.10)$$

gives the dispersion relation

$$\omega^2 = \omega_0^2 q^2 (1 - cq^2), \quad (5.11)$$

as concluded by substituting (5.10) and (5.1) into (5.2)₃ with its right hands-side replaced by $\rho_0 \ddot{u}$. It is also noted that the form (5.11) was obtained by replacing c with $-c$ in (5.1) i.e. by essentially assuming a negative gradient coefficient. This point was not explicitly discussed in the short communication by Altan and Aifantis (1992) where c was effectively assumed negative in order to deduce a value for it consistent with lattice dynamics results [i.e. in order to compare (5.11), also reached by Altan and Aifantis (1992), with a corresponding expression deduced from lattice dynamics arguments]. However, Altan and Aifantis (1992), as well as Ru and Aifantis (1993), used a positive c in order to discuss the solution of crack boundary value problems.

Next, it is shown that the concept of considering a nanostructured material as a mixture of "bulk" and "grain boundary" spaces can also be utilized to model not only its elastic but also its plastic behavior. For example, the well-known "abnormal" flow stress-grain size dependence and its departure from the traditional Hall-Petch equation (Chokshi et al 1992) can be interpreted on the basis of a rule-of-mixtures relationship for the flow stress σ of the form

$$\sigma = f\sigma_G + (1-f)\sigma_{GB}, \quad (5.12)$$

where f denotes the volume fraction of the "bulk" phase and (σ_G, σ_{GB}) the flow stresses of the bulk and grain boundary space. It is further assumed that $\sigma_{GB} = \kappa_0$ is a constant comparable to the flow stress of the amorphous material and that $\sigma_G = \kappa_1 + \beta_1/\sqrt{d}$ obeys the traditional Hall-Petch equation with κ_1, β_1 being constants and d denoting grain diameter. If the nanocrystalline material (in two dimensions) is assumed to consist of square grains of size d_1 separated by the grain boundary space of size δ , it follows that $f = d_1^2/(d_1 + \delta)^2$ and, then, (5.12) becomes

$$\sigma = \frac{1}{(d_1 + \delta)^2} \left[\delta(2d_1 + \delta)\kappa_0 + d_1^2(\kappa_1 + \beta_1/\sqrt{d_1}) \right]. \quad (5.13)$$

Qualitatively, for $d \rightarrow 0$ we have $\sigma = \kappa_0$; for $d \rightarrow \infty$ we have $\sigma = \kappa_1$; while for $\delta = 0$ we have $\sigma = \kappa_1 + \beta_1/\sqrt{d_1}$. Moreover, (5.13) attains a maximum value for $d = d_c$. For $d > d_c$ the traditional Hall-Petch equation holds, while for $d < d_c$ an "inverse" Hall-Petch behavior is obtained. These results verify the experimental observations that the yield strength of traditional materials increases with decreasing grain size until a critical grain size at the nanometer level is reached, after which the yield stress decreases with further decrease of the grain size. Preliminary calculations for nanocrystalline Pd and other metals show a good agreement of (5.13) with the experimental trends. Currently, other models for the shape of the grains (hexagons, spheres etc.) are examined to deduce more elaborate expressions for the volume fraction f but the basic premise depicted in (5.13) is maintained.

Finally, we conclude with some remarks on damage and inelastic deformation for nanostructured materials. Experimental observations pertaining to nanopore formation at triple grain boundary junctions, nanopore

linkage, and nanopore growth by diffusion were reported by Milligan et al (1992). Moreover, some one-dimensional arguments motivated by superplastic flow mechanisms were proposed to obtain a relationship between strain rate and stress including a nanopore-related component. Attention here is focused to the point of view that nanopore growth and migration is an inhomogeneous process and therefore some spatial gradients should be involved. One approach is to begin (Aifantis 1992) with a complete balance law for the nanoporosity ϕ of the form

$$\dot{\phi} + \text{div} \underline{j} = \hat{c} , \quad (5.14)$$

where $\underline{j}$ denotes the flux of nanopores within an elementary volume and $\hat{c}$ denotes nanopore growth and coalescence.

An alternative (and perhaps more suitable) approach would be to employ evolution equations for the vacancy concentration c in the form

$$\dot{c} = D \nabla^2 c + \hat{r}(c, \sigma) , \quad (5.15)$$

and the strain rate $\dot{\epsilon}$ in the form

$$\dot{\epsilon} = E \dot{\sigma} + \hat{g}(c, \sigma) , \quad (5.16)$$

with D being the diffusivity, E being the elastic modulus and $(\hat{r}, \hat{g})$ denoting respectively growth/coalescence of nanopores and production of inelastic strain. Under suitable assumptions for $\hat{r}$ and $\hat{g}$, the adiabatic elimination of the "fast" variable c leads to the following gradient-dependent constitutive equation

$$\dot{\epsilon} = E \dot{\sigma} + \alpha \dot{\sigma} + \beta \sigma^2 + \gamma \nabla^2 \sigma , \quad (5.17)$$

with (α, β, γ) denoting structure-related phenomenological coefficients.

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