TECHNICAL PAPER

Exploring the applicability of gradient elasticity to certain micro/nano reliability problems

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Abstract It has long been assessed that continuum mechanics can be used successfully to address a variety of mechanical problems at both macroscopic and microscopic scales. The term "micromechanics", in particular, has been used in considering elasticity, plasticity, damage, and fracture mechanics problems at the micron scale involving metallic, ceramic and polymeric materials, as well as their composites. Applications to automobile, aerospace, and concrete industries, as well as to chemical and microelectronic technologies have already been documented. The recent developments in the field of nanotechnology have prompted a substantial literature in nanomechanics. While this term was first introduced by the author in the early 90's to advance a generalized continuum mechanics framework for applications at the nanoscale, it is mainly used today in considering "hybrid" ab-initio/molecular dynamics/finite element simulations, usually based on elasticity theory, to interpret the mechanical response of nano-objects (nanotubes, nanowires, nanoaggregates) and extract information on nano-configurations (dislocation cores, crack tips, interfaces). The modest goal of this article is to show that continuum elasticity can indeed be extended to describe a variety of problems at the micro/nano regime. The resultant micro/nanoelasticity theory includes long-range or nonlocal material point interactions and surface effects in the form of (phenomenological) higher-order stress/strain gradients. Coupled thermo-diffuso-chemo-mechanical processes can also be considered within such a higher-order theory. Size effects on micro/nano holes and micro/nano cracks can conveniently be modeled, and some standard strength of materials formulas routinely used for micro/nano beams can be improved, with potential applications to MEMS/NEMS devices and micro/nano reliability components.

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1 Introduction

While multiscale modeling procedures combining atomistic molecular dynamics simulations (based on empirical potentials calibrated or not by ab initio calculations) with finite element computations (usually based on standard elasticity theory) are quite fashionable today, a different modeling approach will be discussed in this paper. This approach is motivated by the desire to properly extend continuum classical elasticity (CE) to address deformation and fracture problems at micron and nano scales in an effective and computationally robust manner. In fact, classical elasticity theory has been used successfully to model the response of certain nanotube configurations and of other nano-objects, in excellent agreement with respective molecular dynamics (MD) simulations (e.g. Ru 2003, and references quoted therein; nonlocal elasticity has been used, among others, by Wang and Hu 2005 and Zhang et al. 2005).

At the same time it is well known that standard mechanics and material science models, which do not contain an internal length scale, fail to provide reasonable results at the micron and nano regimes. A compromise between the CE and MD approaches, which is reasonably suited for problems at the micro/nano transition is the so-

called gradient elasticity theory. This may be viewed as (a special case of) a direct extension of the CE approach to include gradient or nonlocal terms (Aifantis 1978; Triantafyllidis and Aifantis 1986) in the constitutive equations (and sometimes in the balance laws). These terms account for the interaction of length scales (i.e. the scale of the representative elementary volume on which theory and measurement is based upon, and the scale of the underlying material substructure governing the evolution of deformation) as the size of the component or material system under consideration is decreasing.

The interest in higher-order gradient and nonlocal elasticity theories has been revived recently among researchers in various disciplines (solid mechanics, theoretical condensed matter physics, and materials science) due to the ability of the higher-order or nonlocal terms to model phenomena not previously captured by classical elasticity which does not involve an internal length scale in its constitutive structure. Such phenomena include, among other things, the occurrence of size effects (i.e. the dependence of strength or other macroscopic properties on specimen size), as well as fracture and/or interface processes where the detailed "non-singular" or "continuous" distribution of stress and strain fields near the crack tip or the interface is of prime importance. Such distributions of stress/strain fields are extremely useful for the design/ processing and operation of micro/nano devices which often feature geometric singularities or material discontinuities and exhibit size effects.

In this connection it is emphasized that novel experimental mechanics techniques have been developed recently to capture the details of deformation and stress fields near regions of high local strain gradients where application of classical theories predicts singularities (e.g. crack tips) or discontinuities (e.g. interfaces). For this type of experimental work which focuses on capturing the effect of high localized strain gradients, the reader may consult, for example, the work of Sciammarella et al. (2003), and references quoted therein). With respect to the problem of size effect in particular, the author has pointed out in a SEM lecture back in 2000 (Aifantis 2000) to the need of conducting experimental work on microtensile perforated specimens in order to determine the existence of such effects at the micron and submicron scales, in analogy to those observed at the macroscale when the underlying microstructural effects become dominant (e.g. Aifantis 1999, and references quoted therein). This suggestion has been taken up, among others, by Chasiotis who addressed the question of size effects on microtensile perforated specimens in his PhD thesis at Caltech (Chasiotis 2002). Earlier than that, the problem of necking instabilities in polymeric fibers has been considered by him in his Diploma Thesis at Aristotle University by using a simple

version of nonlinear gradient elasticity theory (Chasiotis 1996). More recently, the same author and co-workers have produced very interesting results on both types of problems, i.e. size effects of perforated microtensile MEMS specimens and on stress-strain curves of free-standing thin films (Chasiotis and Knauss 2003; Chasiotis et al. 2007), as discussed later on in this article.

Along similar experimental lines, the theory of gradient elasticity can be used for evaluating possible size effects related to the determination of residual stresses by the microscopic "hole" method as used recently by Michel's group at the Micro-Nano Reliability Center in Berlin. This consists of a hole milling by focused ion beam (FIB) in a thin membrane followed by an evaluation of the stress relief through SEM analysis of the obtained displacement patterns via digital image correlation (DIC). This methodology, which is promoted under the name FibDAC (e.g. Vogel and Michel 2001; Wunderle and Michel 2006; Sabate et al. 2007), is based on classical elasticity solutions for a hollowed thin plate; and, can thus be revisited and modified to include surface stress and gradient-dependent size effects that may be present in such micro/nano configurations. The same holds for related measurements and calculations pertaining to the determination of displacement and stress intensity factors at crack tips.

The plan of the paper is as follows: Sect. 2 provides a brief historical account of higher-order elasticity theories as they were developed in the past (mainly in the 60's) for elastic continua with microstructure and their (ir)relevance to current technology-related applications. Section 3 includes an outline of the author's simplest version of gradient elasticity theory along with a brief discussion for the corresponding phenomenological gradient coefficients (or internal length parameters). Section 4 describes applications of gradient elasticity to certain micro/nano configurations which may be of interest to micro/nano reliability assessment procedures. Finally, Sect. 5 considers briefly extensions of the gradient approach to thermoelasticity and diffusoelasticity problems.

2 Highlights of gradient elasticity theory

2.1 Historical background

An account of recent advances in gradient theory can be found in an article by Aifantis (2003). A partial list of recent references pertaining, in particular, to the so-called strain gradient elasticity theory can be found there, while an account of the early contributions and related references which led to this development can be found in an overview by Altan and Aifantis (1997). Higher-order or generalized theories of elastic continua have been proposed in the 1900's (brothers Cosserat) and later in 1960–1970's (by

Mindlin, Toupin, Eringen, etc.), but these developments involved too many phenomenological coefficients (usually undetermined by microscopic or experimental considerations) and their applicability to real problems was examined mainly in relation to wave propagation studies. In the above mentioned overview, a summary of these early developments can be found, along with a derivation and related applications of the author's a simple gradient elasticity model involving only one extra gradient coefficient. This model is discussed, in particular, with emphasis on the elimination of strain singularities in elastic crack problems, and on vibration/wave propagation studies.

With respect to the application of Cosserat type elastic theories for interpreting size effects in torsion and bending of elastic materials with microstructure (bones, foams), the experimental work of Lakes (Lakes 1983, 1986; Yang and Lakes 1981) deserves to be mentioned. This seems to be the first work undertaking the task of measuring the extra phenomenological coefficients associated with the non-standard higher-order terms. More recent efforts for the experimental determination of gradient coefficients for elastic metallic, polymeric and biological materials, as well as elastic geomaterials with microstructure are described in the work of Aifantis (1999) and Vardoulakis et al. (1998), respectively.

It follows from the above discussion that is desirable, if not necessary, to classify the available gradient elasticity models, discuss the physical origin of the gradient terms and develop suitable experiments for the measurement of the new phenomenological coefficients introduced. This becomes even more demanding in view of recent efforts to employ gradient theory to interpret scale effects and model the deformation and fracture of nanomaterials and components used in micro/nano electronic packaging and other micro/nano technology applications. Progress along these lines is discussed below where, among other things, some microscopic expressions for gradient coefficients and suggestions pertaining to corresponding experiments for their determination are given.

2.2 Outline of the simplest form of gradient elasticity theory

Only the gradient elasticity model (in its simplest form) developed by Aifantis and co-workers will be summarized below. The appropriate constitutive equations for a gradient-dependent elastic deformation (gradient elasticity) may be written as follows:

$$\bar{\sigma}_{ij} = \lambda \bar{\varepsilon}_{\kappa\kappa} \delta_{ij} + 2\mu \bar{\varepsilon}_{ij}; \quad \bar{\sigma}_{ij} = \sigma_{ij} + c_\sigma \nabla^2 \sigma_{ij},$$
$$\bar{\varepsilon}_{ij} = \varepsilon_{ij} + c_\varepsilon \nabla^2 \varepsilon_{ij}, \tag{1}$$

where $(\sigma_{ij}, \varepsilon_{ij})$ denote the stress and strain tensors for elastic deformation. The quantities (λ, μ) are the usual Lamé constants. The gradient coefficients c's are new

phenomenological coefficients to be determined from appropriate experiments and/or appropriate microscopic arguments depending on the prevailing deformation mechanisms and the underlying microstructure. It should be pointed out that the sign and the values of the gradient coefficients c's depend on the deformation state at hand (hardening or softening) and the underlying micro/nano structure. (In fact, the simplest form of gradient elasticity theory corresponds to the case $c_\sigma = 0$.)

As already mentioned, the gradient-elasticity expression of Eq. 1 has been used successfully for interpreting size effects, as well as for eliminating strain singularities from dislocation lines and elastic crack tips (e.g. Aifantis 2003, and references quoted therein). The value of the gradient coefficients may be inferred, in principle, from such measurements pertaining to the extent of dislocation cores and the structure of crack tip opening profiles. Direct estimates for the gradient coefficients may also be obtained from properly designed experiments. For example, pure bending experiments of asymmetrically deforming beams (due to an engineered spatially-inhomogeneous microstructure—e.g. grain size distribution along the beam axis) can provide estimates for the gradient coefficient c_ε in Eq. 1, as this coefficient turns out to relate directly to the (non-constant) radius of curvature of the non-homogeneous beam. Preliminary results have already been reported for the case of plasticity (Aifantis 1992; Murphy et al. 2003) and analogous considerations could be applied, in principle, for elastically bent beams and foils. Theoretical estimates for the gradient coefficient have also been obtained for elastoplastic polycrystals by using self-consistent arguments (Aifantis 1995) and these results can be specialized to elastic deformations to arrive at a proportionality relation between the gradient coefficient $c_\varepsilon \equiv c$ (or internal length) and the grain size d of an elastically deforming polycrystal; i.e., $c \sim A\, d^2$, where the numerical parameter A relates explicitly to the elastic constants of the material in a fashion depending on the self-consistent model used. For random elastic polycrystals the gradient coefficient c turns out to be related to the autocorrelation function $\Lambda(r)$ through the relationship $c \sim B[\partial^2 \Lambda(r)/\partial r^2|_{r=0}]^{-1}$, where B denotes another numerical parameter.

A most exciting but cumbersome evaluation of the gradient coefficient c in the gradient elasticity model of Eq. 1 can be obtained on the basis of recently developed high-resolution optical methods in conjunction with the non-singular solutions obtained for the strain field of dislocation (see, for example, the recent paper by Kioseoglou et al. 2006) and crack problems. This is possible due to the fact that the model of Eq. 1 can estimate the size of dislocation "core" and the size of the "cohesive zone" at crack tips. Other possible estimates for the gradient elasticity coefficient c of Eq. 1 may be obtained from wave propagation

with dispersion studies (see, for example, Altan and Aifantis (1997), and the references quoted therein).

3 Applications to specific micro/nano configurations

In this section we discuss briefly the application of gradient elasticity, as summarized by Eq. 1, to particular problems at the micron and submicron scale range. The specific configurations we examine may be potentially useful to micro/nano technology and micro/nano design and manufacturing.

3.1 Micro/nano beams and plates

Beams and plates of micro/nano dimensions are extensively used as sensors in various micro/nano technology applications, as well as for interpreting experimental measurements for material constants (e.g. elastic moduli) and assessing small scale phenomena (e.g. interfacial/internal stresses). The gradient or micro/nano elasticity relations summarized by Eq. 1, can be used to revisit various classical strength of materials or structural mechanics relationships and derive new modified ones, more suitable for design requirements of micro/nano components and devices.

For example, under certain assumptions, the celebrated Stoney formula may easily be modified (by the second term in the parenthesis in the formula below) to read.

$$\sigma_f = \kappa \frac{\bar{E}_s h_s^2}{6 h_f} \left(1 + \frac{3 c_s}{h_s}\right), \tag{2}$$

where the index f refers to the film and the index s to the substrate, with $(\sigma, \kappa, \bar{E}, h)$ denoting, respectively, film stress, curvature, elastic modulus and thickness. The elastic modulus $\bar{E}_s$ is given by $\bar{E}_s = E_s/(1 - v_s^2)$ - with v_s denoting Poisson's ratio of the substrate—for plane strain conditions, while c_s denotes as usual the relevant gradient coefficient or internal length parameter. It is noted that a variant of the gradient elasticity theory summarized by Eq. 1 has been used for the derivation of Eq. 2. This variant, which includes the first strain gradient as well, arrives at the following expression for the axial beam stress: $\sigma = E[\varepsilon + c \, \text{sign}(\varepsilon)|\nabla \varepsilon|]/(1 - v^2)$ in terms of the axial strain ε and the gradient ∇ along the beam's thickness direction; and, thus, the parameter c has the dimensions of length here. For bending problems within a strength of materials approach, the axial strain distribution is assumed to be linear in the thickness direction; thus, the ∇^2 vanishes and the gradient contribution comes from the ∇ term.

Another example is concerned with the bending of a mirco/nano cantilever beam, as this configuration is relevant, among other things, to the design of actuators and micro/nano probes for chemical and medical applications. A modified expression for the elastic modulus E can easily be derived, under certain conditions, in terms of the displacement δ and the applied load P at the free end of the beam of length L and moment of inertia I. It reads

$$E = \frac{PL^3}{3\delta I} \left[1 + 3 \left(\frac{L}{\sqrt{c}}\right)^{-3} \tan h \left(\frac{L}{\sqrt{c}}\right) - 3 \left(\frac{L}{\sqrt{c}}\right)^{-2}\right]. \tag{3}$$

This formula is derived for appropriate boundary conditions on the basis of a one-dimensional gradient constitutive equation forthe axial stress $\sigma = E(\varepsilon - c\nabla^2 \varepsilon)$, in terms of the axial strain ε and the Laplacian (second derivative along the direction of the beam axis) ∇^2. The coefficient c in this case has the dimensions of length square, as also suggested by Eq. 1.

Typical graphs for σ_f and E corresponding to the above relation are plotted in Fig. 1.

3.2 Nanoscale crack tips

The problem of eliminating the strain singularity from crack tips was addressed within the structure of the simplest form of gradient elasticity theory in Aifantis (1992) (see also Altan and Aifantis 1997); for subsequent
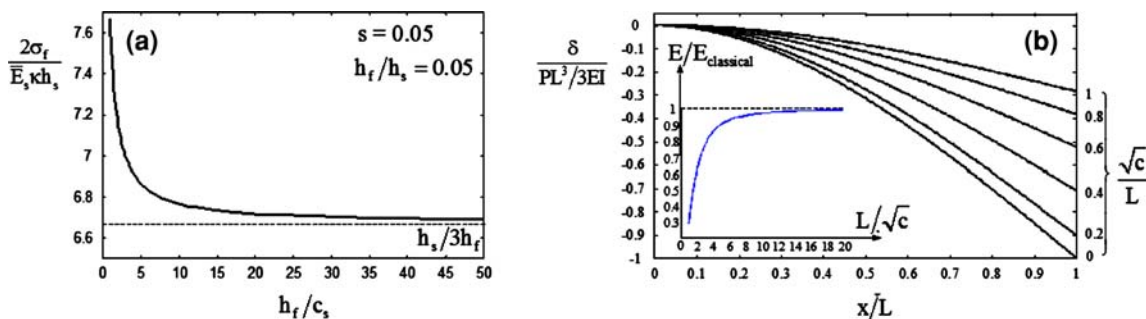

Fig. 1 The effect of gradient coefficient c on (**a**) the internal film stress σ_f as calculated from a gradient modification of Stoney's formula and (**b**) the elastic modulus E as calculated from a gradient modification of a bent cantilever beam by a point load applied at its end

treatments the reader may consult the list of references given in Aifantis (2003). This treatment leads to Barenblatt's "smooth closure condition" for the crack faces without any undesirable property of the strain at the transition boundary between "mathematical" and "physical" crack, and without imposing any cohesive force distribution requirements at the outset. It turns out that the stress singularity may most conveniently be eliminated within the structure of the theory summarized by Eq. 1. This follows from the solution of the inhomogeneous Helmholtz equation

$$(1 - c\nabla^2)\sigma_{ij} = \sigma_{ij}^0, \tag{4}$$

where σ_{ij} is the actual stress field and σ_{ij}^0 is the classical singular elastic stress field.

For the simplest case of a Mode-III crack, it turns out that the only non-vanishing stress components $\sigma_{\alpha 3}$ ($\alpha = 1, 2$) are given by

$$\sigma_{\alpha 3} = \sigma_{\alpha 3}^0 \left(1 - e^{-r/\sqrt{c}}\right), \tag{5}$$

where $\sigma_{13}^0 = -\frac{K_{III}}{\sqrt{2\pi r}}\sin\frac{\theta}{2}$, $\sigma_{23}^0 = \frac{K_{III}}{\sqrt{2\pi r}}\cos\frac{\theta}{2}$, $K_{III} = \tau_\infty\sqrt{\pi a}$, with (r, θ) denoting as usual the polar coordinates from the crack tip, τ_∞ is the applied shear, and a is the half crack length. The stress component σ_{13} distribution in the case of classical and gradient elasticity is shown in Fig. 2.

3.3 Size effects in MEMS

Figure 3 shows a perforated MEMS polycrystalline silicon tensile specimen used by Chasiotis and Knauss (see, for example, Chasiotis and Knauss 2003, and references quoted therein) and the type of perforations used. The parameters K and ρ designate the stress concentration factor and the radius of curvature for each type of perforation used. Figure 4a shows the experimental trends for the strength of each type of perforated specimen used and the corresponding theoretical graph obtained by using gradient elasticity theory is depicted in Fig. 4b. The simplified gradient elastic model used for obtaining these results is given by the constitutive equation.

$$\varepsilon = \frac{1 + v}{E}\sigma - \frac{v}{E}(tr\,\sigma)1 - c\frac{v}{E}\nabla^2(tr\,\sigma)1. \tag{6}$$

The corresponding maximum hoop stress for an infinite plate with a central hole of radius a subjected to uniaxial tension σ reads (v and E denote, as usual, Poisson's ratio and Young's modulus).

$$\sigma_\theta|_{\max} = \sigma\left\{3 - K_0(h)\left[\frac{1}{T_h} + \frac{2(1 + 3v)h}{F_h}\right]\right\}, \tag{7}$$

where, $T_h \equiv hK_1(h) + K_0(h)$, $F_h \equiv 3(1 + v)hK_0(h) + [(1 + v)h^2 + 4]K_1(h)$, $h \equiv a/\sqrt{vc}$, and K_0 and K_1 denote

Fig. 2 Distribution of σ_{13} in Mode-III in the case of: (**a**) Classical elasticity; (**b**) Gradient elasticity

(a)   (b)

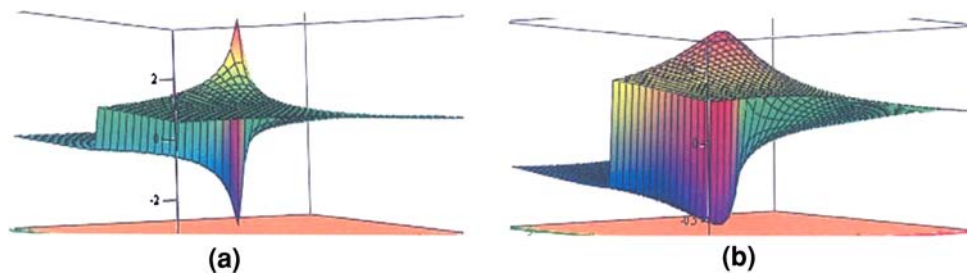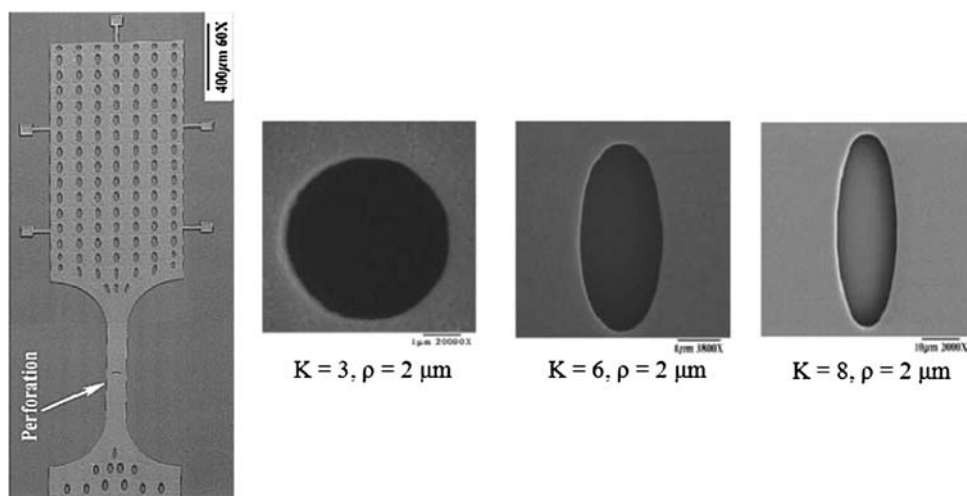**Fig. 3** Perforated MEMS polycrystalline silicon tensile specimen and type of perforation used (Chasiotis 2002; Chasiotis and Knauss 2003)

Perforation

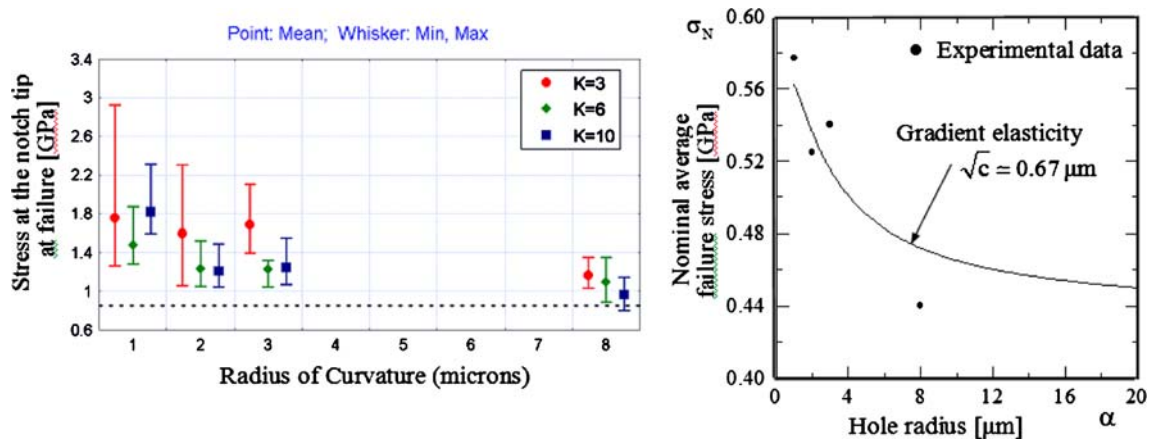K = 3, ρ = 2 μm   K = 6, ρ = 2 μm   K = 8, ρ = 2 μm

Fig. 4 **a** Experimental trends for the strength of each type of perforated specimen used; **b** corresponding theoretical graph obtained by using gradient elasticity theory

Bessel functions of the second kind. If a failure criterion of the form $\sigma_\theta|_{max} = \sigma_c$ (with σ_c denoting a material constant) is adopted, then one obtains the graph depicted in Fig. 4b for $\sigma_c = 0.85$ GPa, $v = 0.22$ and $\sqrt{c} = 0.67\,\mu m$, i.e. an internal length comparable to the average grain size of 0.3 μm of the polysilicon material used.

4 Coupled thermo-chemo-mechanical problems

In this final section an extension of gradient elasticity theory is suggested for coupled thermoelasticity and elastodiffusion problems. Fourier's and Fick's law for heat conduction and mass diffusion may not be applicable for such transports processes at micro/nano scales. Higher-order gradients and nonlocal effects may also be relevant here and a brief discussion of the respective modifications in the constitutive response of stress and heat/diffusion fields is outlined below.

In the case that diffusion of a solute takes place within a deformable elastic solid the stress-strain relation of Eq. 1 is modified as follows

$$\bar{\sigma}_{ij} = \lambda\bar{\varepsilon}_{\kappa\kappa}\delta_{ij} + 2\mu\bar{\varepsilon}_{ij} - \alpha\bar{\rho}\delta_{ij}, \tag{8}$$

where $\bar{\rho}$ is an apparent solute concentration, α is a new phenomenological coefficient and the rest of the symbols are as in Eq. 1. The quantity $\bar{\rho}$ is given by a gradient-dependent constitutive equation analogous to those of Eq. $1_{2,3}$, i.e.

$$\bar{\rho} = \rho + c_\rho\nabla^2\rho, \tag{9}$$

where ρ is the actual local concentration field and c_ρ is a corresponding gradient coefficient measuring nonlocal diffusion effects having the dimension of length square (internal diffusion length).

The evolution of the variable $\bar{\rho}$ may be assumed to obey the uncoupled Fick's law of diffusion, i.e.

$$\partial_t\bar{\rho} = D\nabla^2\bar{\rho}, \tag{10}$$

where D is the macroscopic diffusion coefficient. Eq. 10 can be re-written in terms of the local concentration ρ, giving the following higher-order diffusion equation

$$\partial_t\rho = D\nabla^2\rho - c_\rho\partial_t\nabla^2\rho + Dc_\rho\nabla^4\rho. \tag{11}$$

Various diffusion models are possible depending on the signs of D and c_ρ, as well as the relative magnitude of these constants. When Eq. 11 is combined with Eq. 8 and Eq. $1_{2,3}$ a higher-order fully gradient-dependent but uncoupled elasto-diffusion theory is obtained. It is uncoupled in the sense that the strain or stress field does not enter into the higher-order diffusion equation given by Eq. 1 and, thus, this can be solved first to determine ρ, while the determination of $(\sigma_{ij}, \varepsilon_{ij})$ can be obtained afterwards by combining Eq. 8 with the corresponding equilibrium equation. An uncoupled gradient theory of thermoelasticity may also be obtained in a similar way by replacing the concentration field ρ with the local temperature field θ. Higher-order transport theories of the form discussed herein have first been proposed by the author within a somewhat more general mechanics framework in 1980's (e.g. Aifantis 1980).

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