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LETTER

Comments on "Model and analysis of size-stiffening in nanoporous cellular solids" by Wang and Lam [J. Mater. Sci. 44, 985–991 (2009)]

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Introduction

The mechanical response of microstructured materials can be modelled with sufficient accuracy and efficiently through gradient elasticity. Compared to classical elasticity, the governing equations of gradient elasticity are equipped with additional spatial gradients of relevant variables (such as strains and/or accelerations). Through the inclusion of these additional gradients, phenomena that are dominated by microstructural influences can be modelled accurately and realistically, such as stress and strain concentrations around crack tips [2–5] or dislocation cores [6–8], and the size-dependent mechanical behaviour of specimens [4, 9, 10]. For a more recent account on the use of gradient theory to eliminate elastic singularities in dislocation lines and crack tips, as well as to interpret size effects, one may consult [11]. In dynamics, there is the additional motivation of simulating dispersive wave propagation, but this is beyond the scope of this short note.

Since the partial differential equations (p.d.e.) of gradient elasticity are typically fourth-order equations in terms of displacements, finite element discretisation is usually not straightforward. However, various solutions methods have been suggested and demonstrated. Of particular interest in the context of this short discussion is the solution strategy of Ru and Aifantis, whereby the fourth-order p.d.e. are split into two sets of second-order p.d.e. which can be solved in a decoupled manner [3]. This particular strategy thus enables the use of standard finite element discretisation with continuity of the displacements only [4, 5, 12]. However, it also requires a specific format of the governing equations, in particular, with respect to the constitutive coefficients (or internal length parameters) that accompany the higher-order terms.

Below, we will discuss the particular version of gradient elasticity as developed by Wang and Lam with its finite element implementation. Wang et al. [13] developed a version of gradient elasticity whereby the additional contributions are cast in terms of rotation gradients and the conjugated couple stresses . They have also argued how the solutions of gradient elasticity can be retrieved from the solutions of classical elasticity, see [1] and the follow-up study in [14]. We will discuss their work, in particular, the relation between the solutions of classical elasticity and gradient elasticity. We will also outline amendments that would allow this theory to be implemented via the methodology of Ru and Aifantis.

Construction of gradient elasticity solutions by Wang and Lam

Building on an earlier study [13], Wang and Lam use a particular format of gradient elasticity whereby three groups of higher-order terms are distinguished, related to dilatation, deviatoric stretch, and rotation, respectively. For their particular applications, they chose to include the latter only. This leads to a theory of gradient elasticity with so-called couple stresses, the field equations of which are written as [1, p. 987]

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$$\left(\kappa + \frac{2}{3}\mu\right)u_{j,ij} + \mu u_{i,jj} - \mu\ell_2^2\left(u_{i,jjkk} - u_{j,ijkk}\right) = 0 \quad (1)$$

where u_i are the components of the displacement field, κ and μ are the bulk and shear moduli, ℓ_2 is an internal length scale that accounts for microstructural effects, and indices following a comma denote spatial derivatives.

Wang and Lam then put forth that the equations of conventional elasticity are embedded in Eq. 1, that is

$$\left(\kappa + \frac{2}{3}\mu\right)u_{j,ij} + \mu u_{i,jj} = 0 \quad (2)$$

In particular, they state that "[t]he conventional displacement fields that satisfy this conventional Lamé equation will also satisfy the higher-order equilibrium and governing equations in the bulk of the domain" [1, p. 987]. This was motivated from specific gradient elasticity solutions for beam bending, where the difference between the classical elasticity solution and the gradient elasticity solution was found to be small [13]. However, extrapolating such specific findings to more general geometries and loading cases must be done with extreme care, especially when modelling size effects, since it is well known that the higher-order terms become more and more dominant for smaller and smaller specimen sizes.

Building on their assumption that the solution of classical elasticity is also a solution of gradient elasticity, Wang and Lam suggest to use the classical displacements simply as a surrogate for the gradient displacements: "The recognition of this enables the use of displacement fields that satisfy the conventional Lamé equation as a displacement field template in the development of the higher-order solution" [1, p. 987], and "[t]his means that the higher-order solution and the conventional solution share the same displacement field everywhere except on the boundaries" [14, p. 218].

This is then used to develop a finite element implementation. First, they solve the discrete equations of classical elasticity, after which they use the obtained nodal displacements to compute strain gradients via second-order derivatives of the finite element shape functions [1, p. 988]—thus, one could say that Wang and Lam use the *gradients of classical elasticity*, rather than gradient elasticity. Such an approach would lead to zero strain gradients in case linear finite elements are used (such as three-noded triangles in 2D or four-noded tetrahedrons in 3D), although admittedly Wang and Lam use finite elements with a richer polynomial basis for interpolation.

Critique of the solution strategy of Wang and Lam

We differ with Wang and Lam on two issues, one qualitative and the other quantitative. First, the solutions of classical elasticity and gradient elasticity are fundamentally different, and the former can, in general, not be used as a substitute for the latter. Second, neither can the difference between them be assumed to be small in general; this will depend on the actual size of the problem and the presence of imperfections (dislocations, cracks, notched geometries, etc.) that trigger the gradient activity.

The simple one-dimensional boundary value problem of a shear layer from [11, 15] may serve to illustrate these two points. The shear layer problem is retrieved as a special case from Eq. 1 by letting u_y be the only non-zero displacement component and assuming spatial variations to occur in the x-direction only. Thus, Eq. 1 reduces to

$$\mu u_{y,xx} - \mu\ell_2^2 u_{y,xxxx} = 0 \quad (3)$$

The homogeneous solution of Eq. 3 for classical elasticity (taking $\ell = 0$) reads

$$u_y^{\text{clas}} = A_1 + A_2 x \quad (4)$$

whereas the homogeneous solution for gradient elasticity (taking $\ell \neq 0$) can be written as

$$u_y^{\text{grad}} = B_1 + B_2 x + B_3 \sinh\left(\frac{x}{\ell_2}\right) + B_4 \cosh\left(\frac{x}{\ell_2}\right) \quad (5)$$

Here, the various A_i and B_i are constants that have to be determined via the boundary conditions. In this particular example, the claim of Wang and Lam that the classical elasticity solution satisfies the gradient elasticity differential equation is correct. However, this overlooks the fact that the classical solution is only a *subset* of the gradient solution: the hyperbolic functions in Eq. 5 constitute a clear difference between the solutions of classical elasticity and gradient elasticity and their relative magnitude will be determined by the boundary conditions.

We will assume that no body forces are present, hence the above homogeneous solutions are also the total solutions. The shear layer of length $2L$ with the axis origin placed at the centre is subjected to traction boundary conditions at both ends, that is

$$x = \pm L: \quad \mu\left(u_{y,x} - \ell_2^2 u_{y,xxx}\right) = \bar{\tau} \quad (6)$$

where the quantity on the left-hand-side is the Cauchy shear stress, and a superimposed bar denotes a user-prescribed quantity. Furthermore, for static determinacy we require

$$x = 0: \quad u_y = 0 \quad (7)$$

However, also higher-order boundary conditions are required to solve gradient elasticity boundary value problems. We will use two alternatives, namely, homogeneous natural higher-order boundary conditions as

$$x = \pm L: \quad \mu \ell_2^2 u_{y,xx} = 0 \tag{8}$$

where the quantity on the left-hand-side is the couple stress, and homogeneous essential higher-order boundary conditions as

$$x = \pm L: \quad u_{y,x} = 0 \tag{9}$$

After a bit of straightforward algebra it is found that

$$u_y^{\text{grad}} = \frac{\bar{\tau} x}{\mu} = u_y^{\text{clas}} \tag{10}$$

if Eq. 8 is used, whereas

$$u_y^{\text{grad}} = \frac{\bar{\tau}}{\mu}\left(x - \ell_2 \frac{\sinh(x/\ell_2)}{\cosh(L/\ell_2)}\right) \tag{11}$$

in case Eq. 9 is used (see also [15] for illustration). Figure 1 illustrates the effect of the boundary conditions, as well as the relative magnitude of the material length scale ℓ (the shear strain $\gamma = u_{y,x}$). In this example, the use of vanishing couple stress as the higher-order boundary conditions does not introduce microstructural effects that are absent in the classical solution; however, these boundary conditions do smoothen the singular stress and strain fields that are typically found around crack tips, e.g. [4, 5]. Conversely, using homogeneous essential boundary conditions as the higher-order boundary conditions introduces a boundary layer, the relative importance of which is set by the ratio of the material length scale ℓ_2 over the structural length scale L. For small values of ℓ_2/L the extent of the boundary layer is limited, but for larger values of ℓ_2/L the entire domain may be affected. The ratio ℓ_2/L therefore also determines to what extent the gradient solution differs from the classical solution. For relative small sample sizes, where ℓ_2 is not negligible compared to L, there is a signficant difference between the classical solution and the gradient solution.

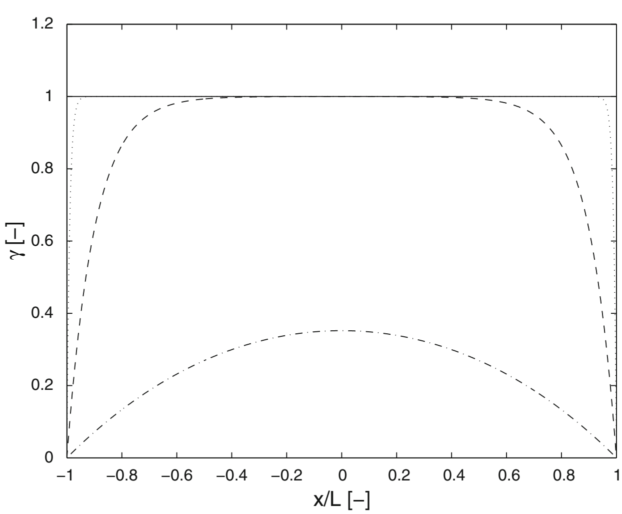

Fig. 1 Shear strain along bar—homogeneous natural boundary conditions (solid), homogeneous essential boundary conditions with $\ell_2 = L/100$ (*dotted*), $\ell_2 = L/10$ (*dashed*) and $\ell_2 = L$ (*dash-dotted*)

The solution strategy of Ru and Aifantis

Despite the criticism expressed above, there is a way forward in using the solution of classical elasticity to construct the solution of gradient elasticity. To this end, the various constitutive coefficients must be related such that it is possible to write the gradient elasticity field equations as

$$\left(\kappa + \frac{2}{3}\mu\right) u_{j,ij} + \mu u_{i,jj} - \ell^2 \left(\kappa + \frac{2}{3}\mu\right) u_{j,ijkk} - \ell^2 \mu u_{i,jjkk} = 0 \tag{12}$$

where ℓ is a generic material length scale. The particular format of Eq. 12 allows to factorise the various derivatives as

$$\left(\kappa + \frac{2}{3}\mu\right) \left[u_j - \ell^2 u_{j,kk}\right]_{,ij} + \mu \left[u_i - \ell^2 u_{i,kk}\right]_{,jj} = 0 \tag{13}$$

The terms in square brackets can be recognised as the classical displacements, that is the displacement components u_i^{clas} satisfying the equations of classical elasticity. Thus, Eq. 13 can be decoupled into two sets of second-order p.d.e. First, one must solve

$$\left(\kappa + \frac{2}{3}\mu\right) u_{j,ij}^{\text{clas}} + \mu u_{i,jj}^{\text{clas}} = 0 \tag{14}$$

for the classical displacements u_i^{clas}, after which this solution is used as a source term in a diffusion-type p.d.e. as

$$u_i^{\text{grad}} - \ell^2 u_{i,jj}^{\text{grad}} = u_i^{\text{clas}} \tag{15}$$

which is to be solved for the gradient displacements u_i^{grad}. This approach has the advantage that standard finite element procedures (with the continuity and polynomial basis of the usual finite element interpolations) can be used for both Eqs. 14 and 15, as this has been explored in [4, 5, 12]. It is also possible to manipulate the associated variationally consistent boundary conditions by taking derivatives of Eq. 15, see for instance [4].

The Ru and Aifantis solution method for gradient elasticity allows to construct gradient elasticity solutions from classical elasticity solutions, provided that the specific format of Eq. 12 is met. It is easy to verify that the particular format of gradient elasticity with rotational gradients only ($\ell_0 = \ell_1 = 0$, $\ell_2 \neq 0$) does not fit the specific formulation of Ru and Aifantis.

In order to be able to cast the couple stress gradient elasticity theory of Wang and Lam in the format of Eq. 12, it is necessary to revisit a more general expression of the field equations [1, p. 987]:

$$\left(\kappa + \frac{2}{3}\mu\right)u_{j,ij} + \mu u_{i,jj} - \mu\left(2\ell_0^2 + \frac{4}{15}\ell_1^2 - \ell_2^2\right)u_{i,jjkk} - \mu\left(\frac{8}{15}\ell_1^2 + \ell_2^2\right)u_{j,ijkk} = 0 \qquad (16)$$

where ℓ_0, ℓ_1 and ℓ_2 are the material length scales related to dilatational gradients, deviatoric stretch gradients and rotational gradients, respectively [13]. In order to match the format of Eq. 12, the higher-order constitutive coefficients must obey the following relation:

$$\frac{\kappa + \frac{2}{3}\mu}{\mu} = \frac{\frac{8}{15}\ell_1^2 + \ell_2^2}{2\ell_0^2 + \frac{4}{15}\ell_1^2 - \ell_2^2} \qquad (17)$$

For general elastic constants κ and μ, it is thus not enough to take $\ell_2 \neq 0$ but $\ell_0 = \ell_1 = 0$; to be able to apply the methodology of Ru and Aifantis one must include dilatational gradients or deviatoric stretch gradients together with the rotational gradients. Nevertheless, such a theory is still applicable to a wide range of materials and phenomena, as we have discussed elsewhere [16].

Conclusions

There is a fundamental difference between the solutions of classical elasticity and gradient elasticity. Moreover, depending on the actual size of the specimen, this difference can be significant from a practical point of view. For relatively large sizes, the effect of the gradient terms is small, and one could indeed use classical elasticity to model such situations—however, without the need to retrieve gradient elasticity solutions from the classical elasticity solutions. On the other hand, for relatively small sizes there may be a significant *qualitative* as well as *quantitative* difference between the solutions of gradient elasticity and classical elasticity.

As we have argued, the basic assumption of Wang and Lam that the classical displacements can be used as a surrogate for the gradient displacements is not valid in general. As an alternative, we suggest the solution strategy of Ru and Aifantis, which is applicable if the three internal length scales of the couple stress gradient elasticity theory employed by Wang and Lam are interrelated as discussed above.

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