Gradient Theory and its Applications to Nanomechanics

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Extended Abstract

Gradient theory, of the form and scope dealt with here, was introduced by the author and his coworkers in the beginning of 1980s to address problems on dislocation patterning, width/spacings of shear bands, and mesh-size independence of finite element calculations in the material softening regime. Prior to that there has been a large number of generalized continuum mechanics theories of gradient type based on mathematical extensions of the Cosserat continuum (multipolar, micropolar, micromorphic, nonlocal media) available in the literature, but they involved a long list of unspecified phenomenological constants and were mainly concerned with wave propagation studies. Thus, the central problem of material instabilities, the emergence and development of deformation patterns and associated plastic heterogeneities were not addressed. In fact, due to the complexity of their mathematical structure, only the linearized version of these theories were used and material softening was excluded. As a result, the aforementioned material instability and inhomogeneity questions could not even be considered within the existing framework of the previously available gradient type theories. The gradient approach discussed here is based on the introduction of length scale effects in elasticity, plasticity and dislocation dynamics by incorporating higher order gradients (often entering in the form of a Laplacian) of strain and/or dislocation densities into the constitutive or evolution equations governing the material description. The resulting models of gradient dislocation dynamics or multi-element defect kinetics, gradient plasticity, and gradient elasticity have been proven very useful in describing dislocation patterning phenomena and the self-organization of structural defects, the width and spacing of shear bands, various types of size effects, as well as the details of the deformation field near dislocation/disclination lines and crack tips. These features could not be captured by classical theory.

In the talk, new advances of gradient theory will be discussed pertaining to the form and origin of gradient terms, as well as the nature and experimental determination of the associated gradient coefficients. Various deformation mechanisms will be assumed giving rise to specific forms of the gradient terms for a large class of problems. Complexity vs. simplicity will be considered in relation to the robustness of these theories to solve outstanding problems of current technology.

In this connection, the general structure of the present formulation will be compared with other gradient type approaches and models published in the literature over the last decade, along with related advantages and disadvantages. An important feature that will be introduced which is not present in any of the previous gradient theories, is

the role of stochasticity. A generic case will be considered for illustrating the competition between stochastic and deterministic gradient effects and its influence on the development of ordered or random heterogeneity along with the implications on the form of the overall stress – strain response.

Emphasis will be placed on illustrating the applicability of gradient theory to interpret the mechanical response of nano–objects including polycrystalline aggregates, multilayered films, nanotubes and nano–biomembranes. Gradient counterparts of standard elasticity, plasticity and fracture mechanisms, formulae that are routinely used to model behavior at the macro and micro scales, will now be derived for corresponding situations at the nanoscale.

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