International Journal of Engineering Science 100 (2016) 74–98

Contents lists available at ScienceDirect

International Journal of Engineering Science

journal homepage: www.elsevier.com/locate/ijengsci

On a second-order rotation gradient theory for linear elastic continua

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ARTICLE INFO

Article history:
Received 22 October 2015
Revised 23 November 2015
Accepted 25 November 2015
Available online 21 December 2015

Keywords:
Higher-order deformation
Rotation gradient
Couple stress
Strain gradient
Linear elasticity

ABSTRACT

A second-order rotation gradient theory for non-classical elastic continua is developed. This theory accounts for the higher-order deformation of the material structure where the material particle inside the elastic domain is idealized as a microvolume having three degrees of freedom, namely, a translation, a micro-rotation, and a higher-order micro-deformation. The associated strain energy density is a function of the infinitesimal strain tensor and the first and second gradients of the rotation tensor. It is demonstrated that for materials in nano-scale applications and because of some defects at the material structure level, a higher-order deformation measure may be needed. The second-strain gradient theory has the merit to account for the higher-order deformation of the material particle. However, this theory has limited applications because it depends on 16 additional material constants for isotropic elastic continua. By discussing some physical concepts relevant to the natures of material structures, crystallinity, and amorphousness, the second-strain gradient theory is reduced to the second-rotation gradient theory for certain types of materials. For isotropic materials, the developed second-rotation gradient theory only depends on three additional material constants instead of 16. A continuum model equipped with an atomic lattice model is then proposed to examine the applicability of the available non-classical theories and the applicability of the proposed theory for different types of materials.

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1. Introduction

In the classical theory of elasticity, a material body is modeled as a continuum. Each material particle is treated as a mass point that has only three translational degrees of freedom. In the classical theory of linear elasticity, the strain energy density is a function of the infinitesimal strain. On the other hand, for micro-/nano-solids, the material particle has to be represented as a small volume element considering its inner structure to describe the microscopic motion and to account for the microstructure size-dependency. Some higher-order micro-continuum theories have been developed to account for the microstructure effects by introducing additional degrees of freedom with additional deformation measures and material constants to the conventional ones (Chen, Lee, & Eskandarian, 2004; Cosserat & Cosserat, 1909; Edelen, 1969; Eringen, 1966, 1999; Eringen & Suhubi, 1964; Hadjesfandiari & Dargush, 2011; Lam, Yang, Chong, Wang, & Tong, 2003; Mindlin, 1964, 1965; Mindlin & Eshel, 1968; Mindlin & Tiersten, 1962; Polyzos & Fotiadis, 2012; Shaat, 2015; Toupin, 1962; Yang, Chong, Lam, & Tong, 2002). These theories are discussed in details in Section 2.

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http://dx.doi.org/10.1016/j.ijengsci.2015.11.009
0020-7225/Published by Elsevier Ltd.

The main motivation that makes scientists in 1960s–1970s develop the non-classical continuum mechanics theories is the inclusion of the higher-orders of the measures of the underlying classical theories from a mathematical point of view (Mindlin, 1964, 1965; Mindlin & Eshel, 1968; Mindlin & Tiersten, 1962; Toupin, 1962). Recently, few researchers have discussed these existing theories from an atomistic point of view (Chen et al., 2004; Polyzos & Fotiadis, 2012). Although these mathematical and atomistic representations show the merit of these non-classical theories to account for the continuum size effects, such as the residuals of the micro-fields and the nonlocal fields, the physical understanding and the applicability of these non-classical continuum theories for different types of materials are absolutely necessary. Due to the lack of the physical understanding of the applicability of the non-classical theories for different materials, these theories have limited contributions to reflect the mechanics of materials in micro-/nano-scale applications. Another reason, the constitutive equations in the context of these non-classical classical theories depend on new material constants which are still experimentally unpredictable. The first contribution of the present study is to bring the suitable physical explanations for the available non-classical continuum theories and their applicability for different types of material structures. With the aid of these explanations, these theories properly can be applied for small-size materials. Furthermore, these explanations can help in investigating the suitable experimental setups to measure the additional constants presented in the context of each theory.

Most of the existing non-classical continuum theories account only for the first-order deformation of the material particle/material structure. However, in some specific cases (see Section 3.1), the higher-order deformation of the material structure has to be accounted for. The necessity to account for the higher-order deformation of the material structure and the way of modeling it are presented as the second contribution of the present paper. A second-order strain gradient theory has been developed such that the strain energy density is a function of the conventional strain in addition to the first and the second gradients of the strain (Mindlin, 1965). This theory is developed based on mathematical concerns to capture some physical phenomena including surface tension and cohesive forces (Mindlin, 1965). In the present effort, the applicability of the second-strain gradient theory for materials without microstructures is discussed. We showed that the second-strain gradient theory has the merit to account for the higher-order deformation of the material particle. For isotropic materials, the second-strain gradient theory has 18 material constants which make it impractical for elastic field problems. To this end, as a third contribution of the present work, a novel linear elasticity theory in which the strain energy density is a function of the infinitesimal strain tensor and the first and second gradients of the rotation tensor is developed. In this theory, the constitutive equations only depend on three additional material constants that make this theory practical for well-defined elastic field problems with the potential to account for the higher-order deformation of the material structure.

This study is organized such that the applicability of the existing micro-continuum theories for different materials is first discussed. Then, the necessity and the modeling of the higher-order deformations of the material structure are investigated. After that, the essential relations of the second-rotation gradient theory are derived and discussed from the continuum and the atomistic points of view representing the limit of application of the theory for materials. The size-dependent linear elasticity for 2D problems, anti-plane problems, and micro/nano beams are then studied. The applicability and the effectiveness of the proposed second-rotation gradient are discussed by comparing the theory to the existing non-classical theories. Finally, a deep discussion on the experimental determination of the additional material constants of the proposed second-rotation gradient theory for different materials is presented.

2. On the applicability of the existing non-classical continuum theories to specific materials

The available non-classical continuum theories and their applicability for materials are presented. A continuum model equipped with an atomic lattice model is proposed to illustrate the microstructure effects on the deformation energy of linear elastic isotropic materials. Moreover, the model is used to map each non-classical continuum theory to the corresponding suitable material type. In the context of continuum mechanics, the material particle inside the continuum represents the main unit of the continuum's material structure. Usually, the material particle represents a single crystal for polycrystalline materials, a single grain for granular materials, or a chain of molecules for amorphous materials. For continua in macro-scale sizes, the material particle (crystal, grain, or chain of molecules) is small enough, compared to the continuum size. Hence, this material particle can be modeled as a mass point and thus the classical theory of elasticity can be applied. On the other hand, when the size of the continuum reduces to micro-/nano-scale sizes, the ratio of the size of the crystal, the grain, or the chain of molecules (material particle) inside the material structure to the size of the continuum increases. Therefore, the material particle should be represented in the context of the continuum theory as a volume element which exceeds the limit of applicability of the classical theories.

The proposed continuum model reveals that the elastic domain of material is considered consisting of an infinite number of material particles and each material particle is a microvolume which has a certain inner structure. To model the inner structure of the material particle, the continuum model is equipped with an atomic lattice model to account for the lattice dynamics of this inner structure. This model is used to show the applicability of the available non-classical micro-continuum theories from the material structure concerns. The material particle is considered as a rigid microvolume, or it is allowed to deform according to the applied micro-continuum theory.

It should be mentioned that the proposed continuum model can be applied to single crystalline materials by considering the whole continuum consisting of a single crystal with the material particle is the unit-cell inside the crystal structure. Thus, by modeling the unit cell as a volume element and considering the internal phonons of the unit cell, the model can reflect the same results as those of molecular dynamics. Moreover, the proposed model can be applied for polycrystalline materials by modeling