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Research paper

Toupin–Mindlin first strain gradient theory revisited for cubic crystals of hexoctahedral class: Analytical expression of the material parameters in terms of the atomic force constants and evaluation via *ab initio* DFT

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ABSTRACT

Capture of the discrete nature of crystalline solids for the purpose of the determination of their mechanical behavior with high precision is of interest. To achieve this objective, two fundamental contributing factors are on top of the list: (1) formulation in the mathematical framework of an appropriate higher order continuum theory rather than using classical treatment, and (2) incorporation of the true anisotropy of the media. The present work revisits Toupin–Mindlin first strain gradient theory for media with general anisotropy, and then specialize it to cubic crystals of hexoctahedral class. This formulation in addition to 3 classical material constants encountered in classical theory of elasticity, gives rise to 11 additional material parameters peculiar to first strain gradient theory. To date, there is no experimental method in the literature for the measurement of these parameters. A methodology incorporating lattice dynamics is proposed, by which all the material parameters including the classic ones are analytically expressed in terms of the atomic force constants. Subsequently, the analytical expressions for the nonzero components of the 4th and 6th order elastic moduli tensors as well as 6 characteristic lengths are derived. Finally, with the aid of *ab initio* calculations all the material properties in Toupin–Mindlin first strain gradient theory are numerically obtained with high precision. In this work the transformation matrices of cubic crystals of diploidal class which also falls under centrosymmetric point groups are discussed as well.

1. Introduction

Design and fabrication of miniature structures, micro- and nano-objects with a desired precision require the incorporation of appropriate highly accurate analysis. It is well-known that, the accuracy of classical continuum theory of elasticity for describing the mechanical behavior of nano-sized structures is insufficient. Moreover, not only its accuracy in the vicinity of the nanoscopic defects deteriorates, but also it is incapable of capturing the size effect of such nono-sized embedded second phase as nano-inhomogeneities and nano-voids. The desire to increase the accuracy of solution through accounting for the discrete nature of matters, turned the attention of some prominent investigators, primarily in the period of about 1960–1975, towards the development of various higher order continuum theories. Despite the fact that such theories, due to their ability to remedy the aforementioned dilemmas, are nowadays in the spotlight, some serious challenges as how to obtain the associated material properties are posed. Herein, we mainly focus on first strain gradient theory for cubic crystals of hexoctahedral class and calculate, in this mathematical framework, all the pertinent material parameters and the components of the elastic moduli tensors.

The first generalization of the classical theory goes back to the nineteenth century. Voigt (1887, 1894) was the first to note that on each face of a differential volume element inside a body, in addition to the action of 3 stress components, there are also 3 moment vectors. Although Voigt's works being the pioneer of this theory, the first comprehensive theory was later presented by Cosserat and Cosserat (1909). In their proposed theory, they assumed that each point, in addition to the 3 translational degrees of freedom considered in classical theory of elasticity, possesses 3 rotational degrees of freedom as well. Appearance of couple stresses in the equations of motion within Cosserat media is a manifestation of consideration of the additional degrees of freedom. In contrast to classical theory of elasticity, it turns out that the pertinent stress tensor for Cosserat media is not symmetric. From a different point of view, each point of a Cosserat

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medium has the degrees of freedom of a rigid body. The orientation of any such point is mathematically representable by the values of a set of 3 orthogonal unit vectors, referred to as "directors" of an "oriented medium" by Ericksen and Truesdell (1957). More generally, if the directors are stretchable and are not restricted to remain mutually orthogonal, then the theory leads to the mechanics of elastic oriented media with "microstructure", considered by Mindlin (1964) for linear elasticity. Toupin (1964) noted that in Cosserat continuum theory, if the rotation of a point is set equal to the local rotation of the medium, then the theory collapses to the couple stress theory of Toupin (1962); Mindlin and Tiersten (1962); Grioli (1960). This theory is also known as "Cosserat theory with constrained rotation", which is a subclass of a more general theory for non-simple materials of grade 2. A material is referred to as "grade N" if the order of the highest position gradient in its energy density function expression is equal to N. For such materials, Toupin (1964) expressed the strain energy density function in terms of 6 components of the strain tensor and 18 components of the first gradient of strain tensor. Toupin's formulation was developed for nonlinear elasticity. The linear version of the theory was presented by Mindlin (1964) in three forms and later elaborately by Mindlin and Eshel (1968) but limited to isotropic media. In the latter work which is developed for isotropic materials, in addition to the usual Lamé constants, λ and μ, gives rise to 5 additional constants and 2 characteristic lengths. Theory of grade 2 materials in Toupin (1964) is referred to as the first strain gradient theory in Mindlin and Eshel (1968). With due attention to the contributions of Toupin (1964); Mindlin (1964), hereafter, theory of grade 2 materials is referred to as "Toupin–Mindlin first strain gradient theory". As it was alluded to, such higher order continuum theories as first strain gradient theory are necessary for a highly accurate analysis near defects and capture of size effect. However, in utilizing these theories, some difficulties arise due to the lack of knowledge about the material properties as well as the challenges for obtaining them. The complication in obtaining all the material parameters worsens if the actual crystal symmetries are appropriately accounted for.

Although, the simplistic assumption of isotropy for the behavior of the existing elements is merely for the convenience of carrying out an analytical solution, for certain problems but not always has led to useful estimates of the actual model. If the principle feature of interest is to capture the effect of the discrete nature of matter with high precision, such a simplistic assumption is not reliable and, hence, accounting for the complete symmetry group of the element of interest is inevitable. The matrix representation of first strain gradient theory for different elastic symmetries was given by Auffray et al. (2013). The main objective of this work is to develop a remedy for the computation of all the material parameters of the cubic crystals of hexoctahedral class that are realized in the mathematical framework of first strain gradient theory. In contrast to the work in Mindlin and Eshel (1968) which has formulated first strain gradient theory for isotropic media, the present work first extends it to general anisotropy, and then simplify the formulation for the case of cubic crystals of hexoctahedral class. It will be shown that, the current formulation falling in this symmetry group results in 3 classical constants and 11 additional material parameters, as oppose to the treatment of Mindlin and Eshel (1968) in which 2 Lamé constants and 5 additional material parameters are involved. The current work gives rise to 6 characteristic lengths in terms of the classical and additional parameters, whereas the latter work involves only 2 characteristic lengths. Furthermore, all the nonzero components of the 4th and 6th order elastic moduli tensors are also represented in terms of the classical and additional parameters. It should be noted that hexoctahedral and diploidal classes are the only two centrosymmetric classes of cubic crystals. Some discussions on the symmetry groups of diploidal class will also be given.

Although, the current work is concerned with the extension of Toupin–Mindlin first strain gradient theory to cubic crystals of hexoctahedral class and the determination of the pertinent material constants, we briefly make note of some contributions on gradient theories for elastic solids. Plasticity is out of the scope of the current study and, hence, to avoid distracting the reader from the main theme we have refrained ourselves from discussing gradient theories on plasticity. A scrutiny of the literature reveals that there are an abundant amount of literature on various forms of gradient elasticity. Much efforts have been given towards the development of simpler versions, so that the corresponding governing equations are more convenient to work with (Altan and Aifantis, 1997; Askes et al., 2002; Lazar and Maugin, 2005; Metrikine and Askes, 2006). Lazar and Po (2015) give a simplified version of first strain gradient theory, but for anisotropic media. For a more comprehensive literature on various simplified versions of gradient theories, one should consult the works of Askes and Aifantis (2011); Cordero et al. (2016); Polizzotto (2017). Establishment of some type of relationships between certain simplified strain gradient continuum and discrete models have also been proposed in the literature (Askes et al., 2002; Metrikine and Askes, 2006). Polyzos and Fotiadis (2012) have related both first and second strain gradient theories in their original forms to an atomistic model except for one-dimensional case. Lam et al. (2003), associated with simplified gradient theory measured the pertinent gradient constants experimentally; the experiments were carried out on the epoxy cantilever beam. Danescu and Grenet (2012), combining continuum and discrete models have obtained the gradient constants of certain gradient theory.

In general, the determination of the material characteristic lengths and additional elastic constants corresponding to any type of higher order mathematical framework via laboratory experimentation is quite tedious. On the other hand, some theoretical approaches which are based on a combination of the higher order continuum theory of interest and the atomistic features of the pertinent crystal have been promising (Shodja and Tehranchi, 2010; Shodja et al., 2012; 2013; Ojaghnezhad and Shodja, 2012; 2013; Admal et al., 2017). This paper aims to present an atomic model of cubic crystals in the context of Toupin–Mindlin strain gradient elasticity and subsequently combined with *ab initio* density functional theory (DFT) calculations, extract the elastic constants and the characteristic lengths for some crystals falling in the hexoctahedral class.

Previously, some theoretical approaches for the calculation of various material parameters pertinent to different continuum theories in their original forms and without any simplifying assumption have been given. For example, Shodja and Tehranchi (2010, 2012) presented an analytical procedure to estimate the characteristic lengths for face-centered cubic (fcc) crystals in first strain gradient theory by utilizing many-body long range Finnis–Sinclair potentials (Finnis and Sinclair, 1984). Shodja et al. (2012) applied this procedure to calculate the additional constants for second strain gradient theory which is suitable for capturing the surface effect. Later, by using *ab initio* DFT calculations (Shodja et al., 2013) determined the elastic constants in first strain gradient theory for isotropic media. In their work the additional constants were related to the elements of Hessian matrix obtained from *ab initio* DFT. Ojaghnezhad and Shodja (2013) employed *ab initio* calculations based on DFT and calculated the additional constants pertinent to the second strain gradient theory for isotropic media. They also calculated the modulus of cohesion and surface energy. Recently, Admal et al. (2017) extended the work of Shodja and Tehranchi (2010) to the case of anisotropic media. Utilizing empirical potentials and first strain gradient theory, they presented some analytical expressions for the corresponding components of the elastic moduli tensors associated with anisotropic media.

The present paper is organized as follows. Section 2 consists of 3 sections. In Section 2.1, the equations of motion, constitutive relations, and boundary conditions are presented for materials with general anisotropy. Section 2.2 discusses the transformation matrices associated with two centrosymmetric classes of cubic crystals. Then the constitutive relations and equations of motion are specialized for cubic crystals of hexoctahedral class. In Section 2.3, for the cubic crystals of