

# 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

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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 4<sup>th</sup> and 6<sup>th</sup> 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.

*Keywords:* first strain gradient theory, cubic crystals of hexoctahedral class, lattice dynamics, atomic force constants, ab initio calculations

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## 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 nano-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 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 \(1962\)](#), and [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,  $\lambda$  and  $\mu$ , 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 \(1964\)](#) and [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 ma-

terial 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 4<sup>th</sup> and 6<sup>th</sup> 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. \(2016\)](#), and [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 exper-

iments 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 subsections. 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 hexoctahedral class, the conditions of positive definiteness of strain energy density function are discussed and some inequalities pertinent to the constraints associated with the classical and additional constants are obtained. In Section 3, the equation of motion as well as the strain energy density function in first strain gradient theory are conformed to the theoretical framework of lattice dynamics. Section 4 consists of subsections 4.1 and 4.2. Section 4.1 is devoted to the analytical derivations of the elastic constants, characteristic lengths, and additional constants in terms of atomic force constants. In Section 4.2 with the aid of ab initio DFT calcula-



tions the elements of the Hessian matrix are obtained for 7 cubic crystals of hexoctahedral class. Subsequently, all the material parameters pertinent to Toupin-Mindlin first strain gradient theory are numerically computed.

## **2. Toupin-Mindlin first strain gradient theory for the cubic crystalline solids: discussion on the associated elastic moduli tensors and the characteristic lengths**

The specialization of the well-known first strain gradient theory of [Toupin \(1964\)](#) to linearly elastic isotropic materials leads to a formulation which is also discussed in the general microstructure theory of [Mindlin \(1964\)](#). In this simplified case, besides the usual Lamé constants, there appear 5 additional constants. These constants give rise to 2 characteristic lengths which enter into the equations of motion. Even under the assumption of isotropy, the experimental measurements of the mentioned additional parameters and characteristic lengths poses serious difficulties. For this reason attention has been given to the theoretical evaluation of these constants, ([Shodja and Tehranchi, 2010](#); [Shodja et al., 2013](#)).

In reality no elements are known to exhibit a truly isotropic behavior. In this section, first strain gradient theory is developed for centrosymmetric cubic crystals of hexoctahedral class which is of importance in a wide range of practical engineering applications. For self-containment, a brief review of first strain gradient for materials with general anisotropy is given in the following section. This will include the introduction of notations and basic equations needed for the subsequent developments given in this work.

### 2.1. First strain gradient theory for anisotropic materials

The most general form of the strain energy density associated with first strain gradient theory is given by:

$$W = b_{ij}\epsilon_{ij} + d_{ijk}\epsilon_{ijk} + \frac{1}{2}c_{ijkl}\epsilon_{ij}\epsilon_{kl} + f_{ijklm}\epsilon_{ij}\epsilon_{klm} + \frac{1}{2}a_{ijklmn}\epsilon_{ijk}\epsilon_{lmn}, \quad (1)$$

in which  $\epsilon_{ij}$  and  $\epsilon_{ijk}$  are the second and third order strain tensors, respectively, and are defined as

$$\epsilon_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) = \frac{1}{2}(u_{i,j} + u_{j,i}), \quad (2a)$$

$$\epsilon_{ijk} = \frac{\partial^2 u_k}{\partial x_i \partial x_j} = u_{k,ij}, \quad (2b)$$

where  $\mathbf{u}$  is the displacement field. The expression for  $\epsilon_{ijk}$  has been represented in 3 different forms by [Mindlin and Eshel \(1968\)](#). Eq. (2b) is the so-called form (I) of first strain gradient theory. Comma “,” in the index denotes differentiation as noted above. Assume that when the strain field is identically zero within the body implies that the stress field is zero, and consequently  $b_{ij} = 0$  and  $d_{ijk} = 0$ .

In Eq. (1),  $c_{ijkl}$  is the traditional 4<sup>th</sup> order elastic moduli tensor and  $f_{ijklm}$  and  $a_{ijklmn}$  are the higher order elastic moduli tensors. For hyper-elastic materials, the corresponding second and third order stress tensors,  $\tau_{pq}$  and  $\mu_{pqr}$  known as Cauchy and double stresses, respectively, are obtained as below:

$$\tau_{pq} = \frac{\partial W}{\partial \epsilon_{pq}} = c_{pqij}\epsilon_{ij} + f_{pqijk}\epsilon_{ijk}, \quad (3a)$$

$$\mu_{pqr} = \frac{\partial W}{\partial \epsilon_{pqr}} = f_{ijpqr}\epsilon_{ij} + a_{pqrjk}\epsilon_{ijk}. \quad (3b)$$

In view of the symmetry of the strain tensors,  $\epsilon_{ij} = \epsilon_{ji}$  and  $\epsilon_{ijk} = \epsilon_{jik}$  it can readily be concluded that:

$$c_{ijkl} = c_{klij} = c_{jikl} = c_{ijlk}, \quad (4a)$$

$$f_{ijklm} = f_{jiklm} = f_{ijlkm}, \quad (4b)$$

$$a_{ijklmn} = a_{lmnijk} = a_{jiklmn} = a_{ijkmln}. \quad (4c)$$

Thus, for hyper-elastic solids the number of the independent components of the elastic moduli tensors,  $\mathbf{c}$ ,  $\mathbf{f}$ , and  $\mathbf{a}$  reduces to 21, 108, and 171, respectively. It should be noted that for the centrosymmetric materials the 5<sup>th</sup> order elastic moduli tensor,  $\mathbf{f}$  vanishes. According to [Mindlin and Eshel \(1968\)](#), in the absence of any body forces the stress equations of motion in the first strain gradient theory has the following form:

$$\tau_{jk,j} - \mu_{ijk,i} = \rho \ddot{u}_k, \quad (5)$$

$$P_k = n_j \tau_{jk} - 2n_j \mathcal{D}_i(\mu_{ijk}) - n_i n_j D(\mu_{ijk}) + \mu_{ijk}(\mathcal{D}_l(n_l)n_i n_j - \mathcal{D}_j(n_i)), \quad (6)$$

$$R_k = n_i n_j \mu_{ijk}, \quad (7)$$

where  $\rho$  is the mass density and  $n_i$  is the  $i$ th-component of the unit normal outward to the surface.  $\ddot{u}_k = \frac{\partial^2 u_k}{\partial t^2}$  is the second derivative of the  $k$ th-component of the displacement field with respect to time.  $P_k$  and  $R_k$  are the  $k$ th-component of the traction and double traction vectors, respectively.  $D$  is the normal derivative defined as:

$$D\psi = n_i \psi_{,i}, \quad (8)$$

and  $\mathcal{D}_i$  is the  $i$ th-component of the surface gradient:

$$\mathcal{D}_i \psi = \psi_{,i} - n_i D\psi. \quad (9)$$

By combining Eqs. (2), (3), and (5), the displacement form of the equations of motion for hyper-elastic centrosymmetric material is obtained:

$$c_{jipq}u_{p,jq} - a_{kjpqr}u_{r,jkpq} = \rho\ddot{u}_i. \quad (10)$$

Mindlin (1968) has obtained the closed-form expansions for the elastic moduli tensors  $\mathbf{c}$  and  $\mathbf{a}$  associated with the cubic crystals of hexoctahedral class. Unfortunately, his representation of the tensor  $\mathbf{a}$  does not have the required symmetry  $a_{ijkpqr} = a_{jikpqr}$ . Its correct form will be derived in the Section 2.2. Mindlin (1968) by comparison of the equations of motion associated with the simple cubic element obtained based on lattice model of Gazis et al. (1960) and those based on first strain gradient theory derives some expressions for the corresponding additional constants in terms of the atomic force constants.

## 2.2. 4<sup>th</sup> and 6<sup>th</sup> order elastic moduli tensors for cubic structures of hexoctahedral class

Mindlin and Eshel (1968) presented the first strain gradient theory for the simplified isotropic materials and introduced 2 characteristic lengths. However, no natural crystals with isotropic structures are known to exist. In this section, first strain gradient theory is developed for the large class of centrosymmetric crystals of cubic structure. It should be noted that centrosymmetric cubic crystals exist in two point groups, hexoctahedral and diploidal indicated by Hermann-Mauguin symbols,  $4/m\bar{3}2/m$  and  $2/m\bar{3}$ , respectively. Let the Cartesian coordinate axes  $x$ ,  $y$ , and  $z$  to coincide with the cubic crystal directions,  $[100]$ ,  $[010]$ , and  $[001]$ , respectively. Based on the order of the Hermann-Mauguin symbols in point groups presented by Tilley (2006), the transformation matrices corresponding to the symmetry elements

of the point groups are  $\mathbf{Q}^I$ ,  $\mathbf{Q}^{II}$ , and  $\mathbf{Q}^{III}$  for diploidal and  $\mathbf{Q}^I$ ,  $\mathbf{Q}^{II}$ ,  $\mathbf{Q}^{III}$ ,  $\mathbf{Q}^{IV}$ , and  $\mathbf{Q}^V$  for hexoctahedral class:

$$\mathbf{Q}^I = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad \mathbf{Q}^{II} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \quad \mathbf{Q}^{III} = \begin{pmatrix} 0 & -1 & 0 \\ 0 & 0 & -1 \\ -1 & 0 & 0 \end{pmatrix},$$

$$\mathbf{Q}^{IV} = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \quad \mathbf{Q}^V = \begin{pmatrix} \cos(\frac{n\pi}{2}) & -\sin(\frac{n\pi}{2}) & 0 \\ \sin(\frac{n\pi}{2}) & \cos(\frac{n\pi}{2}) & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad (11)$$

where  $n$  is an arbitrary integer. According to the Neumann's principle, the symmetry elements associated with the 4<sup>th</sup> and 6<sup>th</sup> order elastic moduli tensors of the crystalline solids include the symmetry elements of the point group of the crystal. The symmetries of the 4<sup>th</sup> and 6<sup>th</sup> order elastic moduli tensors associated with the centrosymmetric cubic crystals are such that:

$$c_{ijkl} = Q_{ip}Q_{jq}Q_{kr}Q_{ls}c_{pqrs}, \quad (12a)$$

$$a_{ijklmn} = Q_{ip}Q_{jq}Q_{kr}Q_{ls}Q_{mt}Q_{nz}a_{pqrstz}. \quad (12b)$$

This work is, in particular, concerned with the centrosymmetric cubic crystals of hexoctahedral class and, thus, in Eqs.(12a) and (12b),  $Q_{ij}$  is an element of the corresponding  $\mathbf{Q}^\alpha$ ,  $\alpha = \text{I, II, } \dots, \text{IV}$ . By accounting for the symmetries of  $c_{ijkl}$  as indicated in Eq. (4a) and the condition (12a), it can be shown that:

$$c_{ijkl} = (\alpha_1 - \alpha_2 - 2\alpha_3)\delta_{ijkl} + \alpha_2\delta_{ij}\delta_{kl} + \alpha_3(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}). \quad (13)$$

That is,  $c_{ijkl}$  has 3 independent constants,  $\alpha_i$ ,  $i = 1, 2, 3$ . In the above expression  $\delta_{ijkl}$  is unity if all indices are equal and zero otherwise. For the

special case where  $\alpha_1 = \lambda + 2\mu$ ,  $\alpha_2 = \lambda$ , and  $\alpha_3 = \mu$  the coefficient of  $\delta_{ijkl}$  vanishes and the resulting expression for  $c_{ijkl}$  corresponds to the isotropic 4<sup>th</sup> order tensor. By the same token, consideration of the symmetries noted in Eq. (4c) and condition (12b) leads to the following expression for the 6<sup>th</sup> order elastic moduli tensor associated with the hexoctahedral class:

$$\begin{aligned}
 a_{ijkpqr} = & a_1(\delta_{ip}\delta_{jr}\delta_{kq} + \delta_{ir}\delta_{jp}\delta_{kq} + \delta_{iq}\delta_{jr}\delta_{kp} + \delta_{ir}\delta_{jq}\delta_{kp}) \\
 & + a_2(\delta_{ip}\delta_{jq}\delta_{kr} + \delta_{iq}\delta_{jp}\delta_{kr}) \\
 & + a_3(\delta_{ik}\delta_{jp}\delta_{qr} + \delta_{ik}\delta_{jq}\delta_{pr} + \delta_{qr}\delta_{jk}\delta_{ip} + \delta_{iq}\delta_{jk}\delta_{pr}) \\
 & + a_4(\delta_{ij}\delta_{kp}\delta_{qr} + \delta_{ij}\delta_{kq}\delta_{pr} + \delta_{jr}\delta_{ik}\delta_{pq} + \delta_{ir}\delta_{jk}\delta_{pq}) \\
 & + a_5(\delta_{ij}\delta_{pq}\delta_{kr}) \\
 & + a_6(\delta_{jq}\delta_{ikpr} + \delta_{jp}\delta_{ikqr} + \delta_{ip}\delta_{jkqr} + \delta_{iq}\delta_{jkpr}) \\
 & + a_7(\delta_{kq}\delta_{ijpr} + \delta_{kp}\delta_{ijqr} + \delta_{jr}\delta_{ikqp} + \delta_{ir}\delta_{jkpq}) \\
 & + a_8(\delta_{kr}\delta_{ijpq}) \\
 & + a_9(\delta_{pq}\delta_{ijkr} + \delta_{ij}\delta_{kpqr}) \\
 & + a_{10}(\delta_{qr}\delta_{ijkp} + \delta_{pr}\delta_{ijkq} + \delta_{ik}\delta_{jpqr} + \delta_{jk}\delta_{ipqr}) \\
 & + a_{11}\delta_{ijkpqr}, \tag{14}
 \end{aligned}$$

where  $\delta_{ijkpqr}$  is unity if all indices are the same and zero otherwise. For materials with general anisotropy, formulation in classical theory involves only the 4<sup>th</sup> order elastic moduli tensor. In contrast, from Eq. (10) it is clear that, formulation in first strain gradient theory, in addition to  $c_{ijkl}$ , gives rise to the 6<sup>th</sup> order elastic moduli tensor,  $a_{ijkpqr}$  as well. This tensor provides further refinement and details about the atomistic structures of the crystal. Now, as seen from Eq. (13) for any cubic crystals the determination of the

components of  $c_{ijkl}$  rests on the calculation of 3 constants,  $\alpha_1$ ,  $\alpha_2$ , and  $\alpha_3$ . But the number of constants on which the components of  $a_{ijkpqr}$  depends upon, varies with the class of the cubic crystals. For example, from Eq. (14) it is seen that for cubic crystals of hexoctahedral class the components of  $a_{ijkpqr}$  are related to 11 independent constants,  $a_1, a_2, \dots, a_{11}$ . Whereas cubic crystals of diploidal class have 17 independent constants; the current work, however, is not concern with this class of crystals. Such constants as  $a_1, a_2, \dots, a_{11}$  which enter the formulation in addition to the constants like  $\alpha_1, \alpha_2$ , and  $\alpha_3$  in classical context, are often referred to as “the additional constants” in the literature. In the present paper, classical and the additional constants will be related to the atomic force constants in lattice dynamics.

By Substitution of Eqs. (13) and (14) into Eq. (10), the equations of motion for the hexoctahedral cubic crystals in the mathematical framework of first strain gradient theory are obtained:

$$\begin{aligned}
 & (\alpha_2 + 2\alpha_3)(1 - l_1^2 \nabla^2)u_{j,ij} - \alpha_3(1 - l_2^2 \nabla^2)(u_{j,ij} - u_{i,jj}) \\
 & - \alpha_3 (l_3^2 u_{n,jklm} \delta_{njklmi} + l_4^2 (u_{j,klmi} \delta_{jklm} + u_{j,jlmn} \delta_{lmni}) + l_5^2 u_{i,jklm} \delta_{jklm}) \\
 & + (\alpha_1 - \alpha_2 - 2\alpha_3)(1 - l_6^2 \nabla^2)u_{j,ik} \delta_{ijk} = \rho \ddot{u}_i,
 \end{aligned} \tag{15}$$

where

$$l_1^2 = \frac{4(a_1 + a_3 + a_4) + 2a_2 + a_5}{\alpha_2 + 2\alpha_3}, \tag{16a}$$

$$l_2^2 = \frac{2a_2 + a_5}{\alpha_3}, \tag{16b}$$

$$l_3^2 = \frac{a_{11}}{\alpha_3}, \tag{16c}$$

$$l_4^2 = \frac{2(a_{10} + a_7)}{\alpha_3}, \tag{16d}$$

$$l_5^2 = \frac{a_8}{\alpha_3}, \quad (16e)$$

$$l_6^2 = \frac{2(2a_6 + a_9)}{\alpha_1 - \alpha_2 - 2\alpha_3}. \quad (16f)$$

In the above relations,  $l_i$ 's,  $i = 1, \dots, 6$  have the dimension of length and are the so-called “characteristic lengths”. It is noteworthy to mention that, for isotropic materials  $a_i = 0$ ,  $i = 6, \dots, 11$ , and consequently the number of nonzero characteristic lengths reduces to just two,  $l_1$  and  $l_2$ .

The elastic constants,  $a_i$ ,  $i = 1, 2, \dots, 11$  and  $\alpha_1$ ,  $\alpha_2$ , and  $\alpha_3$  are not completely arbitrary. The plausible constants are such that the physical condition of thermodynamically stable material subjected to any arbitrary strain field is met.

### 2.3. Positive definiteness of the strain energy density function

With due attention to the discussion in Sections 2.1 and 2.2, for a cubic crystal of hexoctahedral class the strain energy density function (1) reduces to:

$$W = \frac{1}{2}c_{ijkl}\epsilon_{ij}\epsilon_{kl} + \frac{1}{2}a_{ijklmn}\epsilon_{ijk}\epsilon_{lmn}. \quad (17)$$

Using Voigt notation to represent  $\mathbf{c}$  and  $\mathbf{a}$ , the above expression may be rewritten as

$$W = \frac{1}{2}c_{\alpha\beta}x_\alpha x_\beta + \frac{1}{2}a_{\gamma\lambda}y_\gamma y_\lambda, \quad \alpha, \beta = 1, \dots, 6 \quad \text{and} \quad \gamma, \lambda = 1, \dots, 18. \quad (18)$$

in which the strain tensor and its first gradient are represented in the vector forms  $\mathbf{x}$  and  $\mathbf{y}$ , respectively. After some manipulation, Eq. (18) may be



rewritten as:

$$W = \frac{1}{2} \left( \frac{1}{A_1} \xi_1^2 + \frac{1}{A_1 A_2} \xi_2^2 + \cdots + \frac{1}{A_5 A_6} \xi_6^2 \right) + \frac{1}{2} \left( \frac{1}{B_1} \zeta_1^2 + \frac{1}{B_1 B_2} \zeta_2^2 + \cdots + \frac{1}{B_{17} B_{18}} \zeta_{18}^2 \right) \quad (19)$$

where  $\xi_i$ ,  $i = 1, 2, \dots, 6$  and  $\zeta_i$ ,  $i = 1, 2, \dots, 18$  are given in the Appendix. The matrix representations of  $c_{\alpha\beta}$  and  $a_{\gamma\lambda}$ , and their relations, respectively, to  $A_i$ ,  $i = 1, 2, \dots, 6$  and  $B_i$ ,  $i = 1, 2, \dots, 18$  are also given in the Appendix.

The strain energy density function  $W$  given by the expression (19) is positive semidefinite if and only if  $A_i$ ,  $i = 1, 2, \dots, 6$  and  $B_i$ ,  $i = 1, 2, \dots, 18$  are nonnegative. It is positive definite if

$$\alpha_1 > 0, \quad \alpha_1 - \alpha_2 > 0, \quad \alpha_1 + 2\alpha_2 > 0, \quad \alpha_3 > 0, \quad (20)$$

for 4<sup>th</sup> order elastic constants and:

$$a_2 > 0, \quad a_2 - a_1 > 0, \quad a_2 + 2a_1 > 0, \quad (21a)$$

$$d_1 > 0, \quad d_4 - a_5 > 0, \quad d_1 (a_5 + d_4) > 2d_2^2 > 0, \quad (21b)$$

$$(d_4 - a_5) (d_6 - a_3) > (d_5 - a_4)^2 > 0, \quad (21c)$$

$$(a_3 + d_6) \left( d_1 (a_5 + d_4) - 2d_2^2 \right) + (a_4 + d_5) \left( 4d_2 d_3 - d_1 (a_4 + d_5) \right) > 2d_3^2 (a_5 + d_4). \quad (21d)$$

for 6<sup>th</sup> order elastic constants. The constants  $d_1, \dots, d_6$  are linear combinations of the additional elastic constants and are given by Eq. (70) in the Appendix.

Thus far, we have revisited the first strain gradient theory for the cubic crystals of hexoctahedral class and, in this framework, developed the equations of motion, gave the expressions for the 4<sup>th</sup> and 6<sup>th</sup> order elastic moduli tensors, and examined the positive definiteness of the strain energy density function.

The next two sections (Sections 3 and 4) provide two approaches for the determination of the characteristic lengths of the crystals of interest by: 1) comparison of the equations of motion within first strain gradient theory and those of lattice dynamics, and 2) comparison of the strain energy density function within the two frameworks. Moreover, the analytical expression for the additional constants of the crystal which appear in first strain gradient theory, are also obtained by the comparison of the strain energy density function within the two frameworks. An important consequence of this approach is that the obtained expressions show the explicit dependence of the additional constants on the nanoscopic features of the pertinent crystals. To this end, in next section, the equation of motion in first strain gradient theory with general anisotropy is cast into the theoretical framework of lattice dynamics.

### **3. Lattice dynamics representation of first strain gradient theory with general anisotropy**

At first, by using the theory of lattice dynamics, the governing equations of motion of discrete atomic masses located in a perfect crystal of infinite extent are derived. In this framework, the equilibrium position vector of the

$\kappa^{th}$  atom in  $l^{th}$  unit cell is expressed as:

$$\mathbf{r}(l\kappa) = \mathbf{r}(l) + \mathbf{r}(\kappa), \quad (22)$$

where  $\mathbf{r}(l)$  is the position of the  $l^{th}$  unit cell and is written in terms of the lattice vectors,  $\mathbf{a}_1$ ,  $\mathbf{a}_2$ , and  $\mathbf{a}_3$ , and integers  $n_1$ ,  $n_2$ , and  $n_3$  as below:

$$\mathbf{r}(l) = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3, \quad (23)$$

with  $\mathbf{r}(0) \equiv \mathbf{0}$  taken as the origin. The position of the center of the  $\kappa^{th}$  atom within the  $0^{th}$  unit cell is denoted by  $\mathbf{r}(\kappa)$  and is the same for all the unit cells. Suppose that the  $\kappa^{th}$  atom within the  $l^{th}$  unit cell is displaced by an amount  $\mathbf{u}(l\kappa)$ , then its new position denoted by  $\mathbf{R}(l\kappa)$  is given as:

$$\mathbf{R}(l\kappa) = \mathbf{r}(l\kappa) + \mathbf{u}(l\kappa). \quad (24)$$

Assuming that the total potential energy of the crystal is a function of the instantaneous position of the atoms, then by employing Taylor's expansion of energy about the equilibrium, it can be obtained that:

$$\Phi = \Phi_0 + \sum_{l, \kappa} \Phi_i(l\kappa)u_i(l\kappa) + \frac{1}{2} \sum_{\substack{l, \kappa \\ l', \kappa'}} \Phi_{ij}(l\kappa; l'\kappa')u_i(l\kappa)u_j(l'\kappa') + \dots \quad (25)$$

As in the earlier parts of this work, Einstein's summation convention on repeated indices holds. In the above equation,  $\Phi_0$  is the equilibrium potential energy, and

$$\Phi_{ij}(l\kappa; l'\kappa') = \left( \frac{\partial^2 \Phi}{\partial u_i(l, \kappa) \partial u_j(l', \kappa')} \right)_{\mathbf{u}=\mathbf{0}}, \quad (26)$$

is the so-called "atomic force constant". The force acting on the atom ( $l\kappa$ ) in the  $i$ -direction is  $F_i(l\kappa) = -\partial\Phi/\partial u_i(l\kappa)$ . By requiring  $F_i(l\kappa) = 0$  when

$\mathbf{u}(l\kappa) = \mathbf{0}$  for all  $l$  and  $\kappa$ , it implies that  $\Phi_i(l\kappa) = (\partial\Phi/\partial u_i(l\kappa))_{\mathbf{u}=\mathbf{0}} = 0$ . Moreover, by neglecting the higher order terms in the expression (25), it corresponds to the harmonic approximation. Thus, the force acting on the atom ( $l\kappa$ ) in the  $i$ -direction may be given as:

$$F_i(l\kappa) = - \sum_{l', \kappa'} \Phi_{ij}(l\kappa; l'\kappa') u_j(l'\kappa'), \quad (27)$$

in which  $\Phi_{ij}(l\kappa; l'\kappa')$  is interpreted as the negative force exerted on the atom ( $l\kappa$ ) in the  $i$ -direction when the atom ( $l'\kappa'$ ) is given a unit displacement in the  $j$ -direction.

In the framework of lattice dynamics, a perfect crystal is modeled as atomic mass points connected together with springs. Assuming that the mass points interact merely through central forces, the potential energy density of the unit cell can be given as:

$$U(l) = U_0(l) - \frac{1}{4v} \sum_{l', \kappa', \kappa} \Phi_{ij}(l\kappa; l'\kappa') (u_j(l'\kappa') - u_j(l\kappa)) (u_i(l'\kappa') - u_i(l\kappa)), \quad (28)$$

where  $v$  is the volume of the unit cell.  $U_0(l)$  is the potential energy density of the unit cell at a reference equilibrium state and without loss of generality can be dropped out. As it will be shown, the series expression of the potential energy density or equivalent strain energy density of the lattice can be truncated in such a way that it is a function of strain and the first gradient of strain.

As it was alluded to, the aim of this section is to derive the equation of motion within first strain gradient theory with general anisotropy in the framework of lattice dynamics. By assuming that the gradients of displacement field are constant inside the cell, consider Taylor's expansion of the

displacement component  $u_j(l'\kappa')$  for the atom  $(l'\kappa')$  about the atom  $(l\kappa)$ , keeping terms through second order:

$$u_j(l'\kappa') = u_j(l\kappa) + \left. \frac{\partial u_j}{\partial x_m} \right|_{\mathbf{x}=\mathbf{r}(l)} r_m(l'\kappa'; l\kappa) + \frac{1}{2} \left. \frac{\partial^2 u_j}{\partial x_m \partial x_n} \right|_{\mathbf{x}=\mathbf{r}(l)} r_m(l'\kappa'; l\kappa) r_n(l'\kappa'; l\kappa), \quad (29)$$

where  $r_m(l'\kappa'; l\kappa) = r_m(l'\kappa') - r_m(l\kappa)$  is the relative position vector of atoms  $(l'\kappa')$  and  $(l\kappa)$ . Substitution of Eq. (29) into Eq. (28) yields:

$$U(l) = \frac{1}{2} \tilde{c}_{ijmp} \left. \frac{\partial u_j}{\partial x_m} \right|_{\mathbf{x}=\mathbf{r}(l)} \left. \frac{\partial u_i}{\partial x_p} \right|_{\mathbf{x}=\mathbf{r}(l)} + \frac{1}{2} \tilde{c}_{ijmnpq} \left. \frac{\partial^2 u_i}{\partial x_p \partial x_q} \right|_{\mathbf{x}=\mathbf{r}(l)} \left. \frac{\partial^2 u_j}{\partial x_m \partial x_n} \right|_{\mathbf{x}=\mathbf{r}(l)} + \frac{1}{2} \tilde{c}_{ijmnp} \left. \frac{\partial^2 u_j}{\partial x_m \partial x_n} \right|_{\mathbf{x}=\mathbf{r}(l)} \left. \frac{\partial u_i}{\partial x_p} \right|_{\mathbf{x}=\mathbf{r}(l)} + \frac{1}{2} \tilde{c}_{ijmpq} \left. \frac{\partial^2 u_i}{\partial x_p \partial x_q} \right|_{\mathbf{x}=\mathbf{r}(l)} \left. \frac{\partial u_j}{\partial x_m} \right|_{\mathbf{x}=\mathbf{r}(l)}, \quad (30)$$

in which

$$\tilde{c}_{ijmn} = -\frac{1}{2v_a} \sum_{l', \kappa', \kappa} \Phi_{ij}(l\kappa; l'\kappa') r_m(l'\kappa'; l\kappa) r_n(l'\kappa'; l\kappa), \quad (31a)$$

$$\tilde{c}_{ijmnp} = -\frac{1}{4v_a} \sum_{l', \kappa', \kappa} \Phi_{ij}(l\kappa; l'\kappa') r_m(l'\kappa'; l\kappa) r_n(l'\kappa'; l\kappa) r_p(l'\kappa'; l\kappa), \quad (31b)$$

$$\tilde{c}_{ijmnpq} = -\frac{1}{8v_a} \sum_{l', \kappa', \kappa} \Phi_{ij}(l\kappa; l'\kappa') r_m(l'\kappa'; l\kappa) r_n(l'\kappa'; l\kappa) r_p(l'\kappa'; l\kappa) r_q(l'\kappa'; l\kappa). \quad (31c)$$

In the above relations,  $\tilde{c}$ 's may be interpreted as the elastic moduli tensors in lattice dynamics framework. For crystals possessing special symmetries, it can be shown that (Maradudin et al., 1971)

$$\Phi_{ij}(l\kappa; l'\kappa') = Q_{ip} Q_{jq} \Phi_{pq}(LK; L'K'), \quad (32)$$

where  $(l\kappa)$  and  $(l'\kappa')$  is transformed to new lattice sites  $(LK)$  and  $(L'K')$ , respectively.  $Q_{ij}$  is the transformation matrix associated with the crystal point group. Also the position vector  $r_m(l\kappa)$  and  $r_m(l'\kappa')$  are transformed as

$$\begin{aligned} r_m(l\kappa) &= Q_{mt}r_t(LK), \\ r_n(l'\kappa') &= Q_{ns}r_s(L'K'). \end{aligned} \quad (33)$$

Now we have:

$$\begin{aligned} &\Phi_{ij}(l\kappa; l'\kappa')r_m(l'\kappa'; l\kappa)r_n(l'\kappa'; l\kappa) \\ &= Q_{ip}Q_{jq}Q_{mt}Q_{ns}\Phi_{pq}(LK; L'K')r_t(L'K'; LK)r_s(L'K'; LK). \end{aligned} \quad (34)$$

On the other hand, the translational invariant property of crystals implies that:

$$\begin{aligned} \Phi_{pq}(LK; L'K') &= \Phi_{pq}(l\kappa; L' + l - L K'), \\ r_t(L'K'; LK) &= r_t(L' + l - L K'; l\kappa). \end{aligned} \quad (35)$$

By using  $L'$  instead of  $L' + l - L$  just as a change in the notation, we have:

$$\begin{aligned} &\Phi_{ij}(l\kappa; l'\kappa')r_m(l'\kappa'; l\kappa)r_n(l'\kappa'; l\kappa) \\ &= Q_{ip}Q_{jq}Q_{mt}Q_{ns}\Phi_{pq}(l\kappa; L'K')r_t(L'K'; l\kappa)r_s(L'K'; l\kappa). \end{aligned} \quad (36)$$

Summing both sides over all atoms and then divide by  $-2v_a$  yield:

$$\begin{aligned} \tilde{c}_{ijmn} &= -\frac{1}{2v_a} \sum_{l', \kappa', \kappa} \Phi_{ij}(l\kappa; l'\kappa')r_m(l'\kappa'; l\kappa)r_n(l'\kappa'; l\kappa) \\ &= -\frac{1}{2v_a} Q_{ip}Q_{jq}Q_{mt}Q_{ns} \sum_{L', K', K} \Phi_{pq}(l\kappa; L'K')r_t(L'K'; l\kappa)r_s(L'K'; l\kappa) \\ &= \tilde{c}_{pqts}Q_{ip}Q_{jq}Q_{mt}Q_{ns}, \end{aligned} \quad (37)$$

which implies that  $\tilde{c}_{ijmn}$  have the same symmetry point group as  $c_{ijmn}$ , discussed in Section 2.2. Likewise, the same conclusion can be reached for  $\tilde{c}_{ijmnp}$  and  $\tilde{c}_{ijmnpq}$ . For centrosymmetric crystals, the components of the odd-ranked tensors are equal to zero. Hence,  $\tilde{c}_{ijmnp} = 0$  and Eq. (30) becomes:

$$U(l) = \frac{1}{2} \tilde{c}_{ijmp} u_{j,m} u_{i,p} + \frac{1}{2} \tilde{c}_{ijmnpq} u_{i,pq} u_{j,mn}. \quad (38)$$

In fact, by keeping the terms through second order in Eq. (29) has resulted in the appearance of the first as well as second gradients of the displacement components in the strain energy density of lattice given by Eq. (38). The associated medium is referred to as grade 2 material (Toupin, 1964) which in the context of continuum gradient theory is characterized via the strain energy density function given by Eq. (17). As noted earlier, Eq. (17) gives rise to the well-known first strain gradient theory. From Eq. (31a) and according to the symmetry considerations discussed by Huang (1950):

$$\tilde{c}_{ijmn} = \tilde{c}_{jimn} = \tilde{c}_{ijnm} = \tilde{c}_{mnij}. \quad (39)$$

Clearly, from Eq. (31c), it can readily be seen that:

$$\tilde{c}_{ijmnpq} = \tilde{c}_{jimnpq} = \tilde{c}_{ijnmpq} = \tilde{c}_{ijpnmq} = \tilde{c}_{ijqnpm} = \tilde{c}_{ijmpnq} = \tilde{c}_{ijmqpn} = \tilde{c}_{ijmnpq}. \quad (40)$$

Consequently  $\tilde{c}_{ijmn}$  and  $\tilde{c}_{ijmnpq}$  have 21 and 90 independent components, respectively.

For variation of  $\delta u_i$  between fixed limits of  $u_i$  associated with times  $t_0$  and  $t_1$ , Hamilton's principle implies that:

$$\delta \int_{t_0}^{t_1} (\mathcal{T} - \mathcal{W}) dt + \int_{t_0}^{t_1} \delta \mathcal{W}_1 dt = 0, \quad (41)$$

where  $\mathcal{T} = \int_V \frac{1}{2} \rho \dot{u}_j \dot{u}_j dV$  is the total kinetic energy,  $\mathcal{W} = \int_V U dV$  is the total potential energy, and  $\mathcal{W}_1$  is the work done by the external forces. To merge in the result of lattice dynamics theory, the expression for the potential energy density of the unit cell given by Eq. (38) is utilized in  $\mathcal{W} = \int_V U dV$ . Moreover, note that in discrete atomistic arrangements, the mass density of material,  $\rho$  may be represented as:

$$\rho = \frac{1}{v} \sum_{\kappa} m_{\kappa}. \quad (42)$$

The variation of the total potential energy is then obtained as:

$$\begin{aligned} \delta \mathcal{W} &= \int_V \delta U dV = - \int_V (\tilde{c}_{ijmq} u_{j,m} - (\tilde{c}_{ijmnpq} u_{j,mn})_{,p})_{,q} \delta u_i dV \\ &+ \int_V ((\tilde{c}_{ijmq} u_{j,m} - (\tilde{c}_{ijmnpq} u_{j,mn})_{,p}) \delta u_i)_{,q} dV + \int_V (\tilde{c}_{ijmnpq} u_{j,mn} \delta u_{i,p})_{,q} dV, \end{aligned} \quad (43)$$

assuming that the medium is homogeneous and, moreover, bounded by a smooth surface, then by employing the divergence theorem, Eq. (43) becomes:

$$\begin{aligned} \int_V \delta U dV &= - \int_V (\tilde{c}_{ijmq} u_{j,mq} - \tilde{c}_{ijmnpq} u_{j,mnpq}) \delta u_i dV \\ &+ \int_S \tilde{c}_{ijmnpq} [\mathcal{D}_l(n_l) n_p u_{j,mn} n_q - 2n_q \mathcal{D}_p u_{j,mn} - u_{j,mn} \mathcal{D}_p n_q] \delta u_i dS \\ &+ \int_S [\tilde{c}_{ijmq} u_{j,m} n_q - \tilde{c}_{ijmnpq} n_q n_p D u_{j,mn}] \delta u_i dS \\ &+ \int_S \tilde{c}_{ijmnpq} u_{j,mn} n_q n_p D \delta u_i dS, \end{aligned} \quad (44)$$

where  $D$  and  $\mathcal{D}_i$  have been defined in Eqs. (8) and (9), respectively. The variations of the kinetic energy and the total external work are, respectively, given by:

$$\delta \int_{t_0}^{t_1} \mathcal{T} dt = - \int_{t_0}^{t_1} dt \int_V \rho \ddot{u}_k \delta u_k dV, \quad (45)$$



$$\delta\mathcal{W}_1 = \int_S P_k \delta u_k dS + \int_S R_k D(\delta u_k) dS, \quad (46)$$

where  $P_k$  and  $R_k$  have been introduced, respectively, in Eqs. (6) and (7) in the context of first strain gradient theory. Substitution of Eqs. (44), (45), and (46) into Eq. (41), leads to the following equations of motion and the pertinent boundary conditions as below:

$$\tilde{c}_{ijmq} u_{j,mq} - \tilde{c}_{ijmnpq} u_{j,mnpq} = \rho \ddot{u}_i, \quad (47a)$$

$$P_i = \tilde{c}_{ijmnpq} [\mathcal{D}_l n_l n_p n_q u_{j,mn} - 2n_q \mathcal{D}_p u_{j,mn} - u_{j,mn} \mathcal{D}_p n_q - n_q n_p D u_{j,mn}] + \tilde{c}_{ijmq} u_{j,m} n_q, \quad (47b)$$

$$R_i = \tilde{c}_{ijmnpq} u_{j,mn} n_q n_p. \quad (47c)$$

These equations correspond to the lattice dynamics representation of first strain gradient theory with general anisotropy.

#### 4. Determination of the characteristic lengths, 4<sup>th</sup> and 6<sup>th</sup> order elastic moduli tensors of cubic crystals of hexoctahedral class in first strain gradient theory

In Section 4.1, we establish a relation between elastic moduli tensors and the atomic force constants defined in the previous section for crystals with general anisotropy. Subsequently, the results will be specialized for cubic crystals of hexoctahedral class in first strain gradient theory. In Section 4.2, by employing ab initio DFT the characteristic lengths, 4<sup>th</sup> and 6<sup>th</sup> order elastic moduli tensors for several cubic crystals of hexoctahedral class are calculated.

#### 4.1. Analytical formulation

Comparing the equations of motion (47a) and (10), respectively, corresponding to first strain gradient theory within lattice dynamics and continuum frameworks, and using Eqs. (39) and (4a) yields:

$$c_{ijmn} = \tilde{c}_{imjn} + \tilde{c}_{jmin} - \tilde{c}_{jimn}. \quad (48)$$

Likewise, utilizing Eqs. (40) and (4c) leads to:

$$\tilde{c}_{ijmnpq} = \frac{1}{6}(a_{pqimnj} + a_{mqipnj} + a_{mnipqj} + a_{pniqmj} + a_{nqipmj} + a_{pmiqnj}). \quad (49)$$

In general, for hyper-elastic materials  $c_{ijmn}$  has 21 independent constants which can be determined from Eq. (48) since the elements of  $\tilde{c}_{ijmn}$  are given by Eq. (31a) in terms of the atomic force constants. On the other hand,  $\tilde{c}_{ijmnpq}$  has 90 independent components which can be obtained from Eq. (31c), while the 6<sup>th</sup> order elastic moduli tensor,  $a_{ijmnpq}$  has 171 components and, thus, Eq. (49) alone is not sufficient to compute all the elements of  $a_{ijmnpq}$ . Nevertheless, for the case of general anisotropy there are 90 characteristic lengths which are expressible in terms of the components of  $\tilde{c}_{ijmn}$  and  $\tilde{c}_{ijmnpq}$ . The number of characteristic lengths in the case of cubic symmetry of hexoctahedral class reduces to only 6, expressible in terms of  $\tilde{c}_{ijmn}$  and  $\tilde{c}_{ijmnpq}$ . As discussed in Section 3,  $\tilde{c}_{ijmn}$ ,  $\tilde{c}_{ijmnpq}$ ,  $c_{ijmn}$ , and  $a_{ijmnpq}$  belong to the same symmetry point group. Thus, considering Eqs. (48) and (13), it is inferred that:

$$\alpha_1 = \tilde{c}_{3333}, \quad \alpha_2 = 2\tilde{c}_{2323} - \tilde{c}_{2233}, \quad \alpha_3 = \tilde{c}_{2233}. \quad (50)$$

Furthermore, using Eqs. (49), (14), and (16) the following characteristic lengths associated with the crystals having cubic symmetry of hexoctahe-

dral class are obtained:

$$l_1^2 = \frac{12\tilde{c}_{323211} + 3\tilde{c}_{332211}}{\alpha_2 + 2\alpha_3}, \quad (51a)$$

$$l_2^2 = \frac{3\tilde{c}_{332211}}{\alpha_3}, \quad (51b)$$

$$l_3^2 = \frac{\tilde{c}_{333333} - 8\tilde{c}_{323332} - \tilde{c}_{332222} - 6(\tilde{c}_{333322} - 4\tilde{c}_{323211} - \tilde{c}_{332211})}{\alpha_3}, \quad (51c)$$

$$l_4^2 = \frac{4(\tilde{c}_{323332} - 3\tilde{c}_{323211})}{\alpha_3}, \quad (51d)$$

$$l_5^2 = \frac{\tilde{c}_{332222} - 3\tilde{c}_{332211}}{\alpha_3}, \quad (51e)$$

$$l_6^2 = \frac{6(\tilde{c}_{333322} - 2\tilde{c}_{323211} - \tilde{c}_{332211})}{\alpha_1 - \alpha_2 - 2\alpha_3}. \quad (51f)$$

Alternatively, by comparing the energy density function pertaining to first strain gradient theory with that of lattice dynamics, one can calculate not only the characteristic lengths associated with first strain gradient theory but also can compute all the additional constants, 171 constants in the case of general anisotropy and 11 constants in the case of cubic symmetry of hexoctahedral class.

According to the symmetry class discussed in Section 2.2,  $a_{ijmnpq}$  has 11 independent constants for the cubic crystals of hexoctahedral class. The equivalency of the higher order terms in the strain energy density functions pertinent to the two frameworks of lattice dynamics and first strain gradient theory results in:

$$\tilde{c}_{ikjnpq}u_{i,pq}u_{k,jn} = a_{njkpqi}u_{i,pq}u_{k,jn}, \quad (52)$$

which subsequently leads to:

$$a_1 = a_3 = a_4 = \tilde{c}_{323211}, \quad (53a)$$

$$a_2 = a_5 = \tilde{c}_{332211}, \quad (53b)$$

$$a_6 = a_9 = \tilde{c}_{333322} - 2\tilde{c}_{323211} - \tilde{c}_{332211}, \quad (53c)$$

$$a_7 = a_{10} = \tilde{c}_{323332} - 3\tilde{c}_{323211}, \quad (53d)$$

$$a_8 = \tilde{c}_{332222} - 3\tilde{c}_{332211}, \quad (53e)$$

$$a_{11} = \tilde{c}_{333333} - 6\tilde{c}_{333322} - \tilde{c}_{332222} + 6\tilde{c}_{332211} - 8\tilde{c}_{323332} + 24\tilde{c}_{323211}. \quad (53f)$$

**Remark.** *The equivalency of the energy density functions, Eq. (17) for the first strain gradient theory and Eq. (38) for lattice dynamics leads to some consistency conditions between the 4<sup>th</sup> order tensors  $c_{ijkl}$  and  $\tilde{c}_{ijkl}$  and 6<sup>th</sup> order tensors  $a_{ijklmn}$  and  $\tilde{c}_{ijklmn}$ . From this point of view, it can be shown that in addition to the conditions (50), a new constraint reveals as:*

$$\alpha_2 = \alpha_3. \quad (54)$$

*This relation is in accord with the central force hypothesis due to the binary interactions between atoms; in fact, this assumption was incorporated in Eq. (28) followed by Eq. (38). The above equality, Eq. (54) is known as Cauchy relation for cubic crystals.*

#### 4.2. Ab initio calculations

In this section, exploiting the ab initio calculations based on DFT (Hohenberg and Kohn, 1964; Kohn and Sham, 1965), the numerical values of the elements of the 4<sup>th</sup> order elastic moduli tensor,  $\alpha_1$ ,  $\alpha_2$ ,  $\alpha_3$ , and 6<sup>th</sup> order tensor,  $a_1, a_2, \dots, a_{11}$ , as well as the characteristic lengths  $l_1, \dots, l_6$  which appear in the equilibrium equation, (15), are determined for some cubic crystals of hexoctahedral class. Due to the expressions given by Eqs. (50), (51), and (53), all the elastic constants and characteristic lengths are related to the

components of the tensors,  $\tilde{c}_{ijmn}$  and  $\tilde{c}_{ijmnpq}$  which, according to Eqs. (31a) and (31c), are expressed in terms of the atomic force constants and the position of atoms in the relaxed crystal. It can readily be shown that the atomic force constants are equal to the components of the Hessian matrix defined as the second derivatives of the total energy of the crystal with respect to the positions of atoms (Shodja et al., 2013; Ojaghnezhad and Shodja, 2013). Therefore, by calculation of the components of the Hessian matrix of a relaxed crystal, one can evaluate all the 4<sup>th</sup> and 6<sup>th</sup> order elastic moduli tensors of the crystal.

The components of the Hessian matrix of a crystal are numerically determined by using the total-energy and molecular-dynamics Vienna Ab initio Simulation Program (VASP) (Kresse and Hafner, 1993, 1994b; Kresse and Furthmüller, 1996). This program is based on DFT and incorporates plane-wave basis set with ultra-soft pseudopotentials (Kresse and Hafner, 1994a). The kinetic energy cutoff for the plane-wave expansion is considered to be 320 eV. The grid in the first Brillouin zone is selected according to the Monkhorst-Pack (Monkhorst and Pack, 1976) scheme and the exchange-correlation energy is evaluated within the generalized gradient approximation using the Perdew-Burke-Ernzerhof potential revised for solids (Perdew et al., 2008). The components of the Hessian matrix of the crystal energy due to any two atoms ( $l\kappa$ ) and ( $l'\kappa'$ ) are calculated through the central difference method applied to the effective force on the ions. To induce the effective force on the ions, each ion is displaced along each of its degrees of freedom separately, and the effective force on the atom is determined numerically.

By numerical values of the Hessian components at hand, the components

of the 4<sup>th</sup> order elastic moduli tensor are evaluated from Eqs. (31a) and (50). The values of  $\alpha_1$ ,  $\alpha_2$ , and  $\alpha_3$  are calculated for 7 crystalline materials of cubic structures and summarized in Table 1. The available experimental results are given for comparison. It is observed that the results obtained by the present analysis are in agreeable accordance with the experimental counterparts.

Table 1: Fourth order elastic constants of cubic crystals in  $\text{eV}/\text{\AA}^3$  compared with some experimental results available in the literature.

Crystal		$\alpha_1$	$\alpha_2$	$\alpha_3$	Crystal		$\alpha_1$	$\alpha_2$	$\alpha_3$
Cu	present work	1.01	0.64	0.39	C	present work	6.81	0.93	3.74
	exp. 1	1.01	0.76	0.47		exp. 1	5.92	0.94	3.25
	exp. 2	1.10*	0.78*	0.51*		exp. 2	6.72	0.78	3.60
Ni	present work	1.67	0.75	0.63	Si	present work	0.95	0.44	0.63
	exp. 1	1.54	0.92	0.78		exp. 1	1.04	0.40	0.50
	exp. 2	1.63*	0.94*	0.82*		exp. 2	1.04	0.40	0.50
Al	present work	0.66	0.38	0.23	Ge	present work	0.81	0.36	0.58
	exp. 1	0.67	0.38	0.18		exp. 1	0.80	0.30	0.42
	exp. 2	0.71*	0.39*	0.20*		exp. 2	0.80	0.30	0.42
Ca	present work	0.08	0.05	0.09					

Note 1: The experimental data labeled by 1 and 2 is collected from Freund and Suresh (2004) and Kittel (2004), respectively.

Note 2: The superscript \* refers to computations at 0 K.

On the other hand, by applying Eqs. (51) and (53) the characteristic lengths and the elements of the 6<sup>th</sup> order elastic moduli tensor are presented in Tables 2 and 3, respectively.

Table 2: Characteristic lengths for different elements in  $\text{\AA}^2$ .

Crystal	$l_1^2$	$l_2^2$	$l_3^2$	$l_4^2$	$l_5^2$	$l_6^2$
Al	2.18	1.70	-31.87	9.56	3.65	-20.67
Ca	3.08	1.73	-16.54	0.09	0.82	-5.04
Cu	0.34	2.15	-17.15	5.23	-0.10	-9.80
Ni	0.09	0.48	-11.25	3.43	0.41	-14.29
C	0.30	0.95	-8.60	2.64	0.09	-9.23
Ge	3.16	5.38	-2.35	1.31	-2.22	3.89
Si	2.38	3.57	-5.41	1.59	-1.18	1.20

Table 3: Sixth order elastic constants for different elements in  $\text{eV}/\text{\AA}$ .

Crystal	$a_1 = a_3 = a_4$	$a_2 = a_5$	$a_6 = a_9$	$a_7 = a_{10}$	$a_8$	$a_{11}$
Al	0.12	0.13	0.62	0.55	0.84	-7.33
Ca	0.05	0.05	0.13	0.00	0.07	-1.49
Cu	-0.03	0.28	0.67	0.51	-0.04	-6.69
Ni	-0.01	0.10	0.81	0.54	0.26	-7.09
C	-0.09	1.19	2.46	2.47	0.33	-32.14
Ge	0.14	1.04	-0.46	0.19	-1.29	-1.36
Si	0.15	0.75	-0.15	0.25	-0.74	-3.41

### 4.3. Recent developments

As it was alluded to, recently the theoretical determination of the additional constants of crystalline solids within the mathematical framework of first and second strain gradient theories has been the focus of several studies, [Shodja and Tehrani \(2010, 2012\)](#); [Shodja et al. \(2012, 2013\)](#); [Ojaghnezhad and Shodja \(2013\)](#); [Admal et al. \(2017\)](#). These works were briefly discussed in the introduction section. In this section, we draw attention to the comparison between the approaches presented in the current work and [Admal et al. \(2017\)](#) paper. For simple cubic lattices having a one-atom basis, on the ground of the analysis given by [Auffray et al. \(2013\)](#) the nonzero components of the additional elastic constants  $\mathcal{D}_{1,1}$ ,  $\mathcal{D}_{1,2}$ ,  $\mathcal{D}_{1,3}$ ,  $\mathcal{D}_{2,2}$ ,  $\mathcal{D}_{2,3}$ ,  $\mathcal{D}_{2,4}$ ,  $\mathcal{D}_{2,5}$ ,  $\mathcal{D}_{3,3}$ ,  $\mathcal{D}_{3,5}$ ,  $\mathcal{D}_{16,16}$ ,  $\mathcal{D}_{16,17}$  were expressed in terms of the potential energy of each atom by [Admal et al. \(2017\)](#). They utilized form (II) of first strain gradient formulation given by [Mindlin and Eshel \(1968\)](#), while the current work incorporates form (I) of the theory. It can be shown that the additional constants encountered in the work of [Admal et al. \(2017\)](#) are related to those of the current study:

$$\mathcal{D}_{1,1} = 4(a_1 + a_3 + a_4 + a_6 + a_7 + a_{10}) + 2(a_2 + a_9) + a_5 + a_8 + a_{11},$$

$$\mathcal{D}_{1,2} = 4a_3 + 2a_{10} - a_5 - a_9,$$

$$\mathcal{D}_{1,3} = 2a_4 + a_5 + a_9,$$

$$\mathcal{D}_{2,2} = 6a_2 + 4(a_3 + a_6 - a_1 - a_4 - a_7) + a_5 + a_8,$$

$$\mathcal{D}_{2,3} = 4a_1 + 2(a_4 + a_7 - a_2) - a_5 - a_8,$$

$$\mathcal{D}_{2,4} = a_5 + 4(a_3 - a_4),$$

$$\mathcal{D}_{2,5} = 2a_4 - a_5,$$



$$\begin{aligned}
 \mathcal{D}_{3,3} &= 2a_2 + a_5 + a_8, \\
 \mathcal{D}_{3,5} &= a_5, \\
 \mathcal{D}_{16,16} &= 3a_2 - 2a_1, \\
 \mathcal{D}_{16,17} &= 2a_1 - a_2,
 \end{aligned} \tag{55}$$

exactly, where  $a_1, a_2, \dots, a_{11}$  were introduced in Eq. (14). [Admal et al. \(2017\)](#), in the context of their approach examined the effect of several different empirical potentials on the numerical values of the additional elastic constants,  $\mathcal{D}_{1,1}, \mathcal{D}_{1,2}, \dots, \mathcal{D}_{16,17}$  and represented them in a few plots. By the examination of these plots, they realized that, under the assumption of central potential the following conditions hold:

$$\mathcal{D}_{2,4} - \mathcal{D}_{3,5} = 0, \tag{56}$$

$$\mathcal{D}_{2,5} - \mathcal{D}_{16,17} = 0. \tag{57}$$

In the context of the analytical formulation given in the present work, it is shown that in addition to the above conditions three other constraints exist under the assumption of central force interaction:

$$\mathcal{D}_{16,16} + \mathcal{D}_{16,17} - 2\mathcal{D}_{3,5} = 0, \tag{58}$$

$$\mathcal{D}_{1,2} + \mathcal{D}_{1,3} - \mathcal{D}_{2,3} - \mathcal{D}_{3,3} = 0, \tag{59}$$

$$\mathcal{D}_{2,2} + \mathcal{D}_{3,3} + 2\mathcal{D}_{2,3} - 4\mathcal{D}_{1,3} = 0. \tag{60}$$

All five conditions, Eqs. (56)–(60) are derivable analytically by utilizing Eqs. (53a)–(53d) and (55).

In Figs. 1 and 2, the values of the nonzero components of the additional elastic constants obtained for Al and Cu via empirical potentials based calculations by [Admal et al. \(2017\)](#) are compared with the corresponding data

obtained in the present work, based on relations (55) in conjunction with ab initio DFT calculations. It should be emphasized that the data reported by Admal et al. (2017) uses central potential assumption, whereas that of the current study is arrived at by assuming central force interaction. As it is seen from Figs. 1 and 2, Admal et al. (2017) have studied the effect of several embedded-atom methods (EAM) on the values of the constants for Al and Cu. In addition, they also considered the effective medium theory (EMT) for Al. A discussion on the effect of these empirical potentials and the corresponding references are given by Admal et al. (2017).

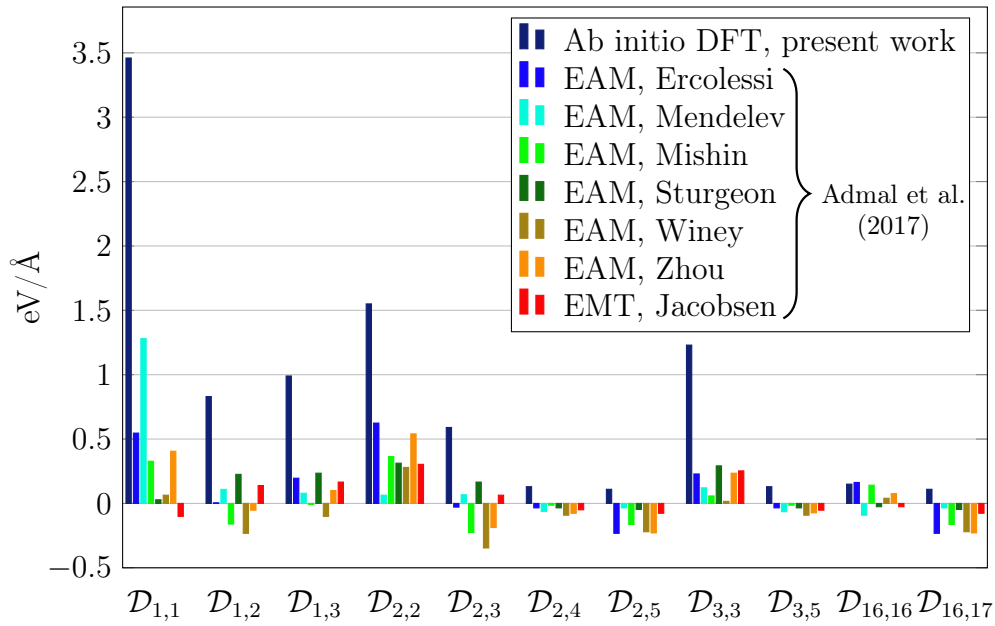


Figure 1: Values of the additional elastic constants for Al obtained by Admal et al. (2017) and the present theory.

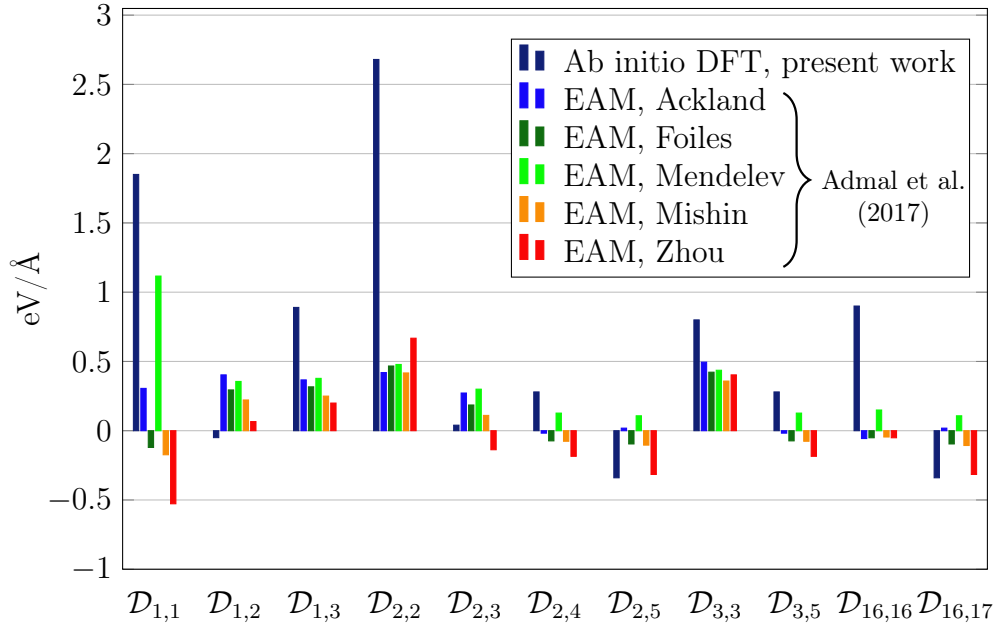


Figure 2: Values of the additional elastic constants for Cu obtained by Admal et al. (2017) and the present theory.

## 5. Conclusion

In this article, first strain gradient theory for hexoctahedral class of cubic crystals including the equations of motion, boundary conditions, and constitutive relations are developed. Moreover, consideration of the positive definiteness of the corresponding strain energy density function led to several inequality constraints on the elements of the 4<sup>th</sup> and 6<sup>th</sup> order elastic moduli tensors. By assuming that the atoms within a crystal interact merely through central forces, a potential energy density function for a unit cell was presented as Eq. (28). Under this hypothesis, and the equivalency of the energies pertinent to the continuum mechanical and lattice dynamics based first strain gradient theories, Cauchy relation was recovered (Remark

of Section 4.1). In contrast to formulation in classical theory which involves the 4<sup>th</sup> order elastic moduli tensor only, formulation in first strain gradient theory gives rise to both, 4<sup>th</sup> and 6<sup>th</sup> order elastic moduli tensors. In fact, the 6<sup>th</sup> order elastic moduli tensor provides a further enhancement and detail on the behavior of the crystal. Consequently, in order to capture the size effect and certain nanoscopic phenomena in various solid mechanics problems of interest, using first strain gradient theory is promising. The 4<sup>th</sup> order elastic moduli tensor for all cubic crystals has 3 independent constants, but distinction in the number of additional constants arise in the components of the 6<sup>th</sup> order elastic moduli tensor. For example, cubic crystals of hexoctahedral and diploidal classes which both are centrosymmetric have, respectively, 11 and 17 independent constants. Obviously, this distinction in the number of nonzero elements which is a reflection on the differences in the atomistic structures of the two crystals provides further details on the behavior of the crystal in response to loadings on a fine scale, beyond those provided by the 4<sup>th</sup> order elastic moduli tensor on a coarse scale. By considering the equations of motion and strain energy density function associated to first strain gradient theory with respect to two different frameworks of continuum and lattice dynamics, followed by the consideration of the pertinent equivalency relations the material parameters consisting of classical constants, characteristic lengths, and additional constants were analytically expressed in terms of the atomic force constants of the crystal. It should be noted that first strain gradient theory of [Mindlin and Eshel \(1968\)](#) was originally developed for isotropic materials, giving rise to only 2 characteristic lengths. In contrast, first strain gradient theory developed herein for the cubic crystals of

hexoctahedral class gives rise to 6 characteristic lengths. By using ab initio based on DFT, the atomic force constants which are equal to the elements of the Hessian matrix are calculated. Subsequently, the numerical values of the additional elastic constants, characteristic lengths, and the components of the 4<sup>th</sup> and 6<sup>th</sup> order elastic moduli tensors of cubic crystals of hexoctahedral class in first strain gradient theory were obtained. The numerical values of these parameters have been calculated for 7 elements which are displayed in Tables 1, 2, and 3. The experimental data for the elastic constants associated to the 4<sup>th</sup> order elastic moduli tensor which are available in the literature are found to be within reasonable agreement of the results obtained in this work. Obtaining the additional constants pertinent to the 6<sup>th</sup> order elastic moduli tensor experimentally, if not impossible would be quite cumbersome.

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### Appendix

In the case of classical elasticity, for cubic crystals of hexoctahedral class, energy density function can be written in Voigt notation as follows:

$$W = \frac{1}{2} \sum_{\beta=1}^6 \sum_{\alpha=1}^6 c_{\alpha\beta} x_{\alpha} x_{\beta}, \quad (61)$$

where the matrix  $\mathbf{x}$  is defined as

$$[x_{\alpha}]_{1 \times 6} = (\epsilon_{11}, \epsilon_{22}, \epsilon_{33}, 2\epsilon_{12}, 2\epsilon_{13}, 2\epsilon_{23}), \quad (62)$$

and with the aid of Eq. (13), the matrix,  $[c_{\alpha\beta}]_{6 \times 6}$  readily leads to

$$[c_{\alpha\beta}]_{6 \times 6} = \begin{pmatrix} \alpha_1 & \alpha_2 & \alpha_2 & & & \\ \alpha_2 & \alpha_1 & \alpha_2 & & & \\ \alpha_2 & \alpha_2 & \alpha_1 & & & \\ & & & \alpha_3 & 0 & 0 \\ & 0 & & 0 & \alpha_3 & 0 \\ & & & 0 & 0 & \alpha_3 \end{pmatrix}. \quad (63)$$

Now the strain energy density function can be rewritten as:

$$W = \frac{1}{2} \left( \frac{1}{A_1} \xi_1^2 + \frac{1}{A_1 A_2} \xi_2^2 + \dots + \frac{1}{A_5 A_6} \xi_6^2 \right), \quad (64)$$

where

$$A_1 = c_{11}, \quad A_2 = \begin{vmatrix} c_{11} & c_{12} \\ c_{21} & c_{22} \end{vmatrix}, \quad A_3 = \begin{vmatrix} c_{11} & c_{12} & c_{13} \\ c_{21} & c_{22} & c_{23} \\ c_{31} & c_{32} & c_{33} \end{vmatrix}, \quad \dots, \quad A_6 = \det([c]_{6 \times 6}). \quad (65)$$

and

$$\begin{aligned} \xi_1 &= \sum_{i=1}^6 c_{1i} x_i, \\ \xi_2 &= \sum_{i=2}^6 (c_{12} c_{1i} - c_{11} c_{2i}) x_i, \\ \xi_3 &= \sum_{i=3}^6 (c_{11} c_{23} c_{2i} + c_{12}^2 c_{3i} + c_{22} (c_{13} c_{1i} - c_{11} c_{3i}) - c_{12} (c_{23} c_{1i} + c_{13} c_{2i})) x_i, \\ &\vdots \end{aligned} \quad (66)$$

It should be mentioned that in the above relations the matrix  $c_{\alpha\beta}$  is a symmetric matrix.

In the similar manner one can rewrite the expression for strain energy density function as mentioned in Eq. (18). In this equation, the matrices  $c_{\alpha\beta}$  and  $\mathbf{x}$  are the same as classical case (62) and (63), and the matrix  $\mathbf{y}$  is defined as

$$[y_\alpha]_{1 \times 18} = (\epsilon_{111}, \epsilon_{221}, \epsilon_{331}, 2\epsilon_{122}, 2\epsilon_{133}, \epsilon_{222}, \epsilon_{112}, \epsilon_{332}, 2\epsilon_{121}, 2\epsilon_{233}, \epsilon_{333}, \epsilon_{113}, \epsilon_{223}, 2\epsilon_{311}, 2\epsilon_{322}, 2\epsilon_{123}, 2\epsilon_{132}, 2\epsilon_{321}). \quad (67)$$

Also by using Eq. (14), the matrix  $a_{\gamma\lambda}$  can be obtained as

$$[a_{\gamma\lambda}]_{18 \times 18} = \begin{pmatrix} [I]_{5 \times 5} & & & 0 \\ & [I]_{5 \times 5} & & \\ & & [I]_{5 \times 5} & \\ 0 & & & [II]_{3 \times 3} \end{pmatrix}, \quad (68)$$

where

$$[I]_{5 \times 5} = \begin{pmatrix} d_1 & d_2 & d_2 & d_3 & d_3 \\ d_2 & d_4 & a_5 & d_5 & a_4 \\ d_2 & a_5 & d_4 & a_4 & d_5 \\ d_3 & d_5 & a_4 & d_6 & a_3 \\ d_3 & a_4 & d_5 & a_3 & d_6 \end{pmatrix}, \quad (69a)$$

$$[II]_{3 \times 3} = \begin{pmatrix} a_2 & a_1 & a_1 \\ a_1 & a_2 & a_1 \\ a_1 & a_1 & a_2 \end{pmatrix}. \quad (69b)$$

In above matrices, constants  $d_1, \dots, d_6$  are:

$$d_1 = 4(a_1 + a_3 + a_4 + a_6 + a_7 + a_{10}) + 2(a_2 + a_9) + a_5 + a_8 + a_{11}, \quad (70a)$$

$$d_2 = a_5 + a_9 + 2a_4, \quad (70b)$$

$$d_3 = a_4 + a_{10} + 2a_3, \quad (70c)$$

$$d_4 = a_5 + a_8 + 2a_2, \quad (70d)$$

$$d_5 = a_4 + a_7 + 2a_1, \quad (70e)$$

$$d_6 = a_1 + a_2 + a_3 + a_6. \quad (70f)$$

Parameters  $\xi_i$ ,  $i = 1, 2, \dots, 6$  and  $A_i$ ,  $i = 1, 2, \dots, 6$  in Eq. (19) are the same as classical one introduced in relations (65) and (66), respectively. If we substitute the matrix  $a_{\gamma\lambda}$  by  $c_{\alpha\beta}$  in (65) and (66) and replace the upper limit of sum in (66), 6 by 18,  $\zeta_i$ ,  $i = 1, 2, \dots, 18$  and  $B_i$ ,  $i = 1, 2, \dots, 18$  can be obtained too. Therefore, all parameters appeared in Eq. (19) are determined.

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