Journal of the Brazilian Society of Mechanical Sciences and Engineering (2019) 41:351
https://doi.org/10.1007/s40430-019-1849-x

TECHNICAL PAPER

Vibration analysis of Love nanorods using doublet mechanics theory

Ufuk Gul[1] · **Metin Aydogdu**[1]

Received: 26 March 2019 / Accepted: 23 July 2019 / Published online: 2 August 2019
© The Brazilian Society of Mechanical Sciences and Engineering 2019

Abstract
Longitudinal vibration of a nanorod is investigated based on the doublet mechanics theory with Love's assumption. By using Hamilton's principle, governing equation and corresponding boundary conditions are derived. Exact frequency equations are obtained for clamped–clamped and clamped-free boundary conditions. Obtained results are compared to the classical elasticity model, other size-dependent nonlocal theories and molecular dynamics simulation. The effects of the length scale parameter, rod length and lateral inertia are investigated.

Keywords Doublet mechanics · Lateral inertia · Love theory · Nanorod · Vibration

1 Inroduction

One-dimensional (1-D) nanostructures like carbon nanotubes, nanoropes, nanofibers, nanorods, nanowires, etc., have attracted a lot of interest due to their excellent electrical and mechanical properties. These 1-D nanostructures have been used in nano-electro-mechanical systems as a nanosensor, nanoactuator, nanomotor and as fibers in new-generation advanced composite structures. Different models have been developed in order to investigate the statics and dynamics of macro- and nanorods. The first and the simplest rod theory has been developed by Bernoulli [1] for longitudinal vibration in the eighteenth century. This theory is firstly used for the analysis of 1-D wave propagation and vibration of thin rods. Only axial deformation effect is included in the classical rod model. Then, Rayleigh [2] proposed a rod theory which considers the lateral inertia in axial vibration of the rods. Love further developed this theory which is now called as Love rod theory [3]. It is noted that the lateral inertia effects are significant for rods with low length/diameter ratio (aspect ratio, L/d). Governing equation of the Love theory shows that lateral inertia effects depend on the Poisson's ratio. In this theory, radial deformation has been expressed in terms of axial deformation. In this way, this theory has one degree of freedom in terms of displacement field and it is called as uni-modal theory in some cases. By taking Poisson's ratio or radius of gyration as zero in governing equation of the Love theory, classical rod theory can be obtained.

Although classical theories are adequate for the static and dynamic analyses of the thin macro-rods, they are not useful for short micro-/nanoscale rods due to existing size effects at nanolength scale. For this reason, some size-dependent continuum models have been developed using higher gradients of the strain or stress gradient. Aydogdu [4] studied the longitudinal vibration of a nanorod using the nonlocal rod theory. Han et al. [5] studied the vibrational energy flow of the rods considering the lateral inertia effects. Wave propagation in a nonlocal nanorod model is investigated by Narendar [6]. It is obtained that unlike classical theory nonlocal model predicts dispersive wave propagation similar to lattice dynamics and experimental results. Moreover, the propagation of longitudinal stress waves has been studied via modified couple stress theory in [7]. Recently, Li et al. [8] studied the longitudinal vibration of a nanobar carrying a nanoparticle using the nonlocal elasticity theory. The lateral inertia effects have been taken into account in their analysis. Another remarkable study is related to axial wave propagation and vibration of nonlocal nanorods with Bishop's assumption [9]. Radial inertia and deformation are both considered, and nonlocal scale parameter effect has been shown in that paper.

In the aforementioned papers, dynamics of a nanorod generally has been analyzed with the nonlocal elasticity, the

Technical Editor: José Roberto de França Arruda.

✉ Metin Aydogdu
metina@trakya.edu.tr

[1] Department of Mechanical Engineering, Trakya University, 22030 Edirne, Turkey

strain gradient elasticity and the modified couple stress models. Except these scale-dependent theories, doublet mechanics (DM) is another alternative micro-mechanics theory which was developed by Granik [10] and it was applied for mechanical modeling of the granular materials in [11]. The main difference of DM from the other scale-dependent model is the definition of the internal length scale parameter. In DM, bonding length of atoms in the considered material is taken as a length scale parameter. In contrast to DM, the determination of the internal length scale parameter in the other size-dependent continuum models is an open problem. Therefore, these size-dependent continuum models can be considered as phenomenological models. They include a great number of phenomenological macro-constants which cannot be defined by experiments. In the DM theory, micro-stresses and micro-strains are defined as vectors, and then these micro-relations are transformed to macro-stress–macro-strain relations. Doublet stress component in the present DM theory represents the microforces and microcouples of the directional particle interactions, adequately. The DM is reformulated for a finite-element approach by Kojic et al. [12]. Longitudinal vibration of the nanorods embedded in an elastic matrix has been studied by considering the DM theory coupled with classical rod model by the present authors [13]. Obtained results using DM model were compared with the classical elasticity theory in this paper. Gul and Aydogdu [14] studied static and dynamic analyses of the nanorods and nanobeams investigated via the DM theory and classical rod theory and Euler–Bernoulli beam model. The results predicted by the DM theory have been compared to the nonlocal elasticity, strain gradient model and experiment for validation. It was shown that the best agreement of the experimental results was obtained for the DM theory in nanorod. Vajari and Imam [15, 16] studied the torsional and axial vibration of the single-walled carbon nanotubes based on the DM theory. Furthermore, flexural vibration and buckling of nanofibers have been studied via DM model in [17]. Elastic medium effects have been considered in that paper. The main difference of the present study from the aforementioned articles related to DM theory is investigation of the lateral inertia effect on the dynamic analysis of a DM nanorod model. To the best knowledge of the authors, this is the first theoretical investigation of the vibration of the Love nanorod model using the DM theory. As it is known, during the axial vibration, extension or shrinking is observed along the longitudinal direction of a rod. Then, expansion or contraction that occurs along the radial direction of the nanorod is accompanied by axial lengthening or shortening of the rod [3]. This modification on the classical rod theory has been considered in the Love theory by considering transverse displacement in the kinetic energy of the rod (since each material point of the rod has a transverse velocity). High precision and sensitivity are crucial for the design of the nanorods. So, radial deformation which is related to lateral inertia should be considered in the design of the nanorods with high radius-to-length ratios and for high frequency numbers.

The objective of the present article is to study the axial free vibration of a nanorod considering the lateral inertia effects (Love's assumption) based on the DM theory. After a brief review of the DM, the governing equation and classical and non-classical boundary conditions are derived via Hamilton's principle by taking the lateral inertia effect. Corresponding natural frequencies are obtained for clamped–clamped and clamped-free boundary conditions. The influences of the rod length, mode number, length scale parameter and lateral inertia on the natural frequencies of nanorods are discussed in detail. Obtained results are compared with the other nonlocal models and molecular dynamics simulation for validation.

2 Formulation for doublet mechanics model

The DM theory is a multi-scale theory which bridges between the lattice dynamics at the nanoscale and continuum mechanics at the macroscale limit. Any pair of neighboring nodes is called as doublet, and they are located at a separation distance $\eta_\alpha = |\xi_\alpha|$. For the present study, each doublet undergoes an elongation ϵ_α and the shear micro-strain and torsional micro-strain of the doublets can also be considered. For each doublet, the increment of displacement in scalar form can be defined as [11]:

$$\Delta u_\alpha = \sum_{\chi=1}^{M} \frac{(\eta_\alpha)^\chi}{\chi!} \tau^o_{\alpha k_1} \dots \tau^o_{\alpha k_\chi} \frac{\partial^\chi u_i}{\partial \chi_{k_1} \dots \partial \chi_{k_\chi}} \tag{1}$$

where each of the subscripts $k_1, \dots k_\chi$ are integer which take values of 1, 2 and 3 corresponding to three-dimensional Cartesian coordinates, M is the number of terms in Taylor series expansion which shows the discreteness of the solid and τ^o_α is the unit vector in α direction. In this work, we consider the first three terms ($M=3$) in the Taylor series expansion while defining the micro-strains and micro-stresses in the solid. By taking $M=1$ in the Taylor series expansion, the classical elasticity theory is obtained. The elongation micro-strain ϵ_α in the α-doublet is defined as [11]:

$$\epsilon_\alpha = \tau^o_{\alpha_i} \sum_{\chi=1}^{M} \frac{(\eta^o_\alpha)^{\chi-1}}{\chi!} \tau^o_{\alpha k_1} \dots \tau^o_{\alpha k_\chi} \frac{\partial^\chi u_i}{\partial \chi_{k_1} \dots \partial \chi_{k_\chi}} \tag{2}$$

where superscript ^{o} refers to the initial configuration of the system. For $M=3$, micro-strain is

$$\epsilon_\alpha = \tau^o_{\alpha i} \tau^o_{\alpha j} \frac{\partial u_i}{\partial x_j} + \tau^o_{\alpha i} \frac{\eta_\alpha}{2} \tau^o_{\alpha j} \tau^o_{\alpha k} \frac{\partial^2 u_i}{\partial x_j \partial x_k} + \tau^o_{\alpha i} \frac{\eta^2_\alpha}{6} \tau^o_{\alpha j} \tau^o_{\alpha k} \tau^o_{\alpha l} \frac{\partial^3 u_i}{\partial x_j \partial x_k \partial x_l} \tag{3}$$

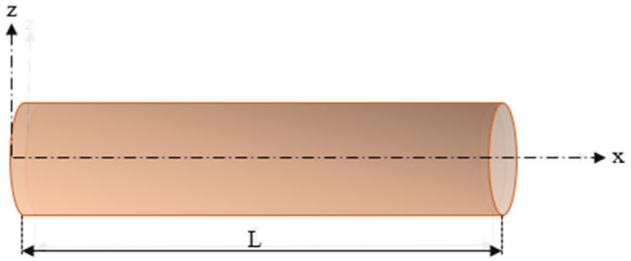

Fig. 1 A nanorod model

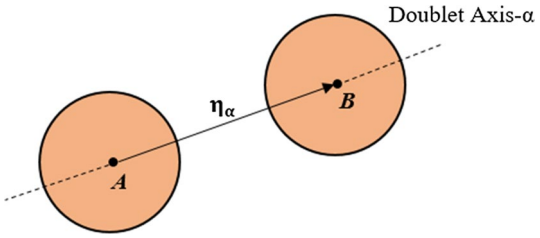

Fig. 2 Schematic diagram of doublet in a solid

The micro-stress p_α and the micro-strain ϵ_α relations are given as

$$p_\alpha = \sum_\beta B_{\alpha\beta}\epsilon_\beta \tag{4}$$

where $B_{\alpha\beta}$ denotes the matrix of micro-modulus of the doublet between the nodes α and β and ϵ_β denotes the axial micro-strain associated with β doublet. The matrix of micro-elastic modulus $B_{\alpha\beta}$ is defined in terms of the Lamé's constants in the previous papers [14, 17]. For this study, we utilize the nanorod model shown in Fig. 1.

The relationship between micro-stress and macro-stress can be defined as [11]:

$$\sigma^{(M)}_{k_1 i} = \sum_{\alpha=1}^{m} \tau^o_{\alpha k_1} \sum_{\chi=1}^{M} (-1)^{\chi+1} \times \left[\frac{(\eta_\alpha)^{\chi-1}}{\chi!} \tau^o_{\alpha k_2} \ldots \tau^o_{\alpha k_\chi} \frac{\partial^{\chi-1} p_{\alpha i}}{\partial \chi_{k_2} \ldots \partial \chi_{k_\chi}} \right] \tag{5}$$

It is noted that these macro-/micro-stress relations are gradually presented in Appendix A. Using $p_{\alpha i} = p_\alpha \tau^o_{\alpha i}$, Eq. (5) takes the following form for $M=1$:

$$\sigma_{ij} = \sum_{\alpha=1}^{m} \tau^o_{\alpha i} \tau^o_{\alpha j} p_\alpha \tag{6}$$

where m is the number of the adjacent nodes in the doublet. And for $M=3$, macro-stress and micro-stress relations are

$$\sigma^{(M)}_{ij} = \sum_{\alpha=1}^{n} \tau^0_{\alpha i} \tau^0_{\alpha j} \left\{ \left(p_\alpha - \frac{1}{2}\eta_\alpha \vec{\tau}^{\,0}_\alpha . (\nabla p_\alpha) + \frac{1}{6}\eta^2_\alpha \left[\left(\vec{\tau}^{\,0}_\alpha . \nabla \right) \left(\vec{\tau}^{\,0}_\alpha . \nabla p_\alpha \right) \right] \right) \right\} \tag{7}$$

Applying the plane stress condition and considering the only axial strain, stress expression in DM theory can be obtained as

$$\sigma^M_{xx} = E\left(\varepsilon_{11} + \frac{1}{12}\eta^2 \frac{\partial^2 \varepsilon_{11}}{\partial x^2} \right) \tag{8}$$

where E is the elasticity modulus of the considered material, ε_{11} is the classical strain component and η is the doublet separation distance which represents distance of both atoms in doublet (Fig. 2), and it denotes bonding length of atoms in the considered solid. It is seen that the first term of Eq. (8) is the classical Cauchy stress and the second term of Eq. (8) is the doublet stress in the present DM theory. It should be noted that stress expression in Eq. (8) is obtained for zigzag type nanorod model. Moreover, obtaining stress expression for armchair nanorod model is given in Appendix.

3 Governing equation and boundary conditions of a Love nanorod model

Consider a nanorod of length L and diameter d. Let u and w denote the displacement along the nanorod length and radial directions, respectively. According to Love theory, the radial deformation of a typical point of nanorod is $w = -r\nu u'$. Where r is the radial position of the point and ν is the Poisson's ratio. A typical point of rod with nonzero r moves not only in the axial direction as seen in the classical model, but also in the radial direction. Plane sections remain plane during the deformation of the rod. The governing equation and boundary conditions for a nanorod can be obtained by using Hamilton's principle:

$$\int_{t_0}^{t_1} \delta(U - T - W)\mathrm{d}t = 0 \tag{9}$$

where δ is the variational operator, T is the kinetic energy, U is the total strain energy stored during the deformation of the nanorod and W is the total work done by external forces. The strain energy can be expressed as [13]:The strain energy of the nanorod can be defined as

$$U_s = \frac{1}{2}\int_0^L [\tau.\varepsilon - \mu.\nabla\varepsilon]\mathrm{d}x \tag{10}$$

where

$$\tau = \nabla\varepsilon = \mathrm{d}\varepsilon/\mathrm{d}x \quad \tau = Eu', \quad \mu = \frac{\eta^2}{12}Eu''. \tag{11}$$

$$u' = \frac{\partial u}{\partial x}, \quad u'' = \frac{\partial^2 u}{\partial x^2}. \tag{12}$$

Thus, the strain energy becomes as follows

$$U = \frac{1}{2}\int_0^L AE\left[(u')^2 - \frac{\eta^2}{12}(u'')^2\right]\mathrm{d}x \tag{13}$$

a time derivative. In addition, the first variation of the total work done by external forces is given by

$$\int_{t_0}^{t_1}\delta W\mathrm{d}t = \int_{t_0}^{t_1}\int_0^L f(x,t)\delta u\mathrm{d}x\mathrm{d}t + \int_{t_0}^{t_1}\left\{[N\delta u]_0^L + \left[R\delta u'\right]_0^L\right\}\mathrm{d}t \tag{15}$$

where f denotes the distributed force, N denotes the concentrated force and R denotes double force (force couple). Inserting Eqs. (13–15) into Eq. (9), variational equation for the nanorod takes the following form:

$$\int_{t_0}^{t_1}\int_0^L\left[AE\left(u'' + \frac{\eta^2}{12}u^{IV}\right) + f - \rho A\ddot{u} + \rho\nu^2 I_\mathrm{p}\left(\ddot{u}''\right)^2\right]\delta u\mathrm{d}x\mathrm{d}t + \int_{t_0}^{t_1}\left[\left\{N - AE\left(u' + \frac{\eta^2}{12}u'''\right) - \rho\nu^2 I_\mathrm{p}\left(\ddot{u}'\right)^2\right\}\delta u\right]_0^L\mathrm{d}t$$
$$+\int_{t_0}^{t_1}\left[\left\{R - AE\left(-\frac{\eta^2}{12}u''\right)\right\}\delta u'\right]_0^L\mathrm{d}t + \int_0^L\left[\rho A\dot{u}\delta u\right]_{t_0}^{t_1}\mathrm{d}x = 0 \tag{16}$$

where the first and second terms are the contribution of the classical elasticity and DM theories, respectively. It should be noted that Ferrari et al. [11 (in pp. 158)] have shown that strain energy of continuum in terms of micro-stress and micro-strain is positive definite. However, its macro counterpart given in Eq. (10) may be unstable due to negative sign of the second term. Similar behavior has been observed in the strain gradient model with positive sign proposed by [13, 18].

The kinetic energy of the rod can be defined as

$$T = \frac{1}{2}\int_0^L\left[\rho A(\dot{u})^2 + \rho\nu^2 I_\mathrm{p}\left(\dot{u}'\right)^2\right]\mathrm{d}x \tag{14}$$

where L is length of the nanorod, A is the cross-sectional area, ρ is the mass density, ν is the Poisson's ratio, and I_p is the polar moment of inertia of the nanorod. The first and second terms of the integral in Eq. (14) correspond to the kinetic energy due to longitudinal and radial motion. Thus, we have considered the radial inertia for the vibration of the nanorod based on the DM theory. This leads to the Love rod theory coupled with the DM. It is noted that dot (.) describes

From Eq. (16), the equation of motion of the nanorod, initial conditions and boundary conditions can be obtained, respectively.

$$AE\left[(u''(x,t) + \frac{\eta^2}{12}u^{IV}(x,t)\right] + f - \rho A\ddot{u}(x,t) + \rho\nu^2 I_\mathrm{p}\ddot{u}''(x,t) = 0 \tag{17}$$

Equation (17) shows the equation of motion of a nanorod based on the DM model with Love's assumption. The last term of Eq. (17) is related to lateral inertia of the nanorod. If the last term of Eq. (17) is set to zero, the nanorod theory for the DM model is obtained [13]. Furthermore, if the last term and the scale parameter $\frac{\eta^2}{12}$ are neglected, Eq. (17) reduces to the classical rod theory.

Initials conditions are obtained as

$$\dot{u}(x,t_1)\delta u(x,t_1) - \dot{u}(x,t_0)\delta u(x,t_0) = 0 \tag{18}$$

Lastly, boundary conditions are

$$\left[N(L,t) - AE\left[u'(L,t) + \frac{\eta^2}{12}u'''(L,t) - \rho\nu^2 I_\mathrm{p}\ddot{u}'(L,t)\right]\right]\delta u(L,t) - \left[N(0,t) - AE\left[u'(0,t) + \frac{\eta^2}{12}u'''(0,t) - \rho\nu^2 I_\mathrm{p}\ddot{u}'(0,t)\right]\right]\delta u(0,t) = 0,$$
$$\left[R(L,t) - AE\left[-\frac{\eta^2}{12}u''(L,t)\right]\right]\delta u'(L,t) - \left[R(0,t) - AE\left[-\frac{\eta^2}{12}u''(0,t)\right]\right]\delta u'(0,t) = 0 \tag{19}$$

In Eq. (19), four boundary conditions are obtained for the longitudinal motion of the nanorod. It is seen that two classical boundary conditions are displacement, u, and the axial force, $AE\left[u' + \frac{\eta^2}{12}u''' - \rho\nu^2 I_\mathrm{p}\ddot{u}'\right]$, respectively. In addition, the non-classical boundary conditions are boundary strain u'

Table 1 Deformation states of different rod theories

Theory	Deformation state			
	Axial deformation	Axial inertia	Doublet strain gradient	Lateral inertia
Classical	✓	✓		
Love	✓	✓		✓
Classical DM	✓	✓	✓	
DM with Love assumption	✓	✓	✓	✓

and the boundary double force $AE\frac{\eta^2}{12}u''$ for the present DM model. By discarding the lateral inertia terms (setting $\nu = 0$ or $I_p = 0$) in Eq. (19), boundary conditions are obtained for the DM nanorod model. By ignoring both the lateral inertia terms and length scale parameter in Eq. (19), we can get the boundary conditions for the simple rod theory.

4 Vibration analysis of the DM nanorod models with Love's assumption

Longitudinal free vibration of nanorods considering the lateral inertia effects has been analyzed using the DM theory in this section. Based on the separation of variables method, longitudinal displacement *u(x,t)* can be expressed as

$$u(x,t) = U(x)e^{i\omega t} \tag{20}$$

where U is the amplitude and ω (rad/s) is the natural frequency of the nanorod. Substitution of Eq. (20) into Eq. (17) without a uniformly distributed load ($f=0$) leads to

$$\beta^2 U^{IV} + \left(1 - \Omega^2 r_g^2 \nu^2\right)U'' + \Omega^2 U = 0 \tag{21}$$

To simplify the analysis, dimensionless variables are defined in the following form

$$\beta^2 = \frac{\eta^2}{12L^2}, \Omega^2 = \frac{\rho\omega^2 L^2}{E}, r_g^2 = \frac{I_p}{AL^2}, \bar{x} = \frac{x}{L}. \tag{22}$$

Here, r_g denotes the radius of gyration of the nanorod. Contribution of the different terms given in Eq. (21) is presented in Table 1 considering their deformation states. When β and ν (or r_g) equal to zero, classical rod equation of motion is obtained. This equation contains the axial deformation and axial inertia. Classical Love theory can be obtained by taking ν and r_g as nonzero. In this case, axial deformation, axial inertia and lateral inertia effects are included. When β is nonzero and ν (or r_g) equal to zero, classical doublet rod equation of motion is obtained. This theory includes the axial and lateral inertias and doublet strain gradient. And the last case includes all effects given in Table 1.

The analytical solution of Eq. (21) can be written as

$$U(\bar{x}) = c_1 \sin\gamma\bar{x} + c_2 \cos\gamma\bar{x} + c_3 \sin\theta\bar{x} + c_4 \cos\theta\bar{x} \tag{23}$$

where c_i ($i=1,2,3,4$) are undetermined coefficients and

$$\gamma = \sqrt{\frac{\left(1 - \Omega^2 r_g^2 \nu^2\right) + \sqrt{\left(1 - \Omega^2 r_g^2 \nu^2\right)^2 - 4\beta^2\Omega^2}}{2\beta^2}},$$
$$\theta = \sqrt{\frac{\left(1 - \Omega^2 r_g^2 \nu^2\right) - \sqrt{\left(1 - \Omega^2 r_g^2 \nu^2\right)^2 - 4\beta^2\Omega^2}}{2\beta^2}}. \tag{24}$$

For a clamped–clamped (C–C) nanorod, the classical and non-classical boundary conditions can be written in dimensionless form as follows

$$\text{Clamped end} \ : \ U(\bar{x}) = 0 \ \ \text{(classical)}, \quad U(\bar{x})'' = 0 \ \ \text{(non-classical) at } \bar{x} = 0, 1. \tag{25}$$

By using the boundary conditions and equation of motion (Eqs. 23, 25), following relation can be obtained

$$\begin{bmatrix} 0 & 1 & 0 & 1 \\ 0 & -\gamma^2 & 0 & -\theta^2 \\ \sin(\gamma) & \cos(\gamma) & \sin(\theta) & \cos(\theta) \\ -\gamma^2\sin(\gamma) & -\gamma^2\cos(\gamma) & -\theta^2\sin(\theta) & -\theta^2\cos(\theta) \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \\ c_3 \\ c_4 \end{bmatrix} = 0 \tag{26}$$

For a non-trivial solution of Eq. (26), the determinant of the coefficient matrix in Eq. (26) has to vanish. This gives the frequency equation of the C–C nanorod model

$$-\left(\gamma^2 - \theta^2\right)^2 \sin(\gamma)\sin(\theta) = 0 \tag{27}$$

Solution Eq. (27) corresponds to natural frequencies of the DM nanorod model with Love's assumption

$$\Omega = \frac{n\pi\sqrt{-(n\pi\beta - 1)(n\pi\beta + 1)\left(n^2\pi^2 r_g^2 \nu^2 + 1\right)}}{n^2\pi^2 r_g^2 \nu^2 + 1} \tag{28}$$

It should be noted that the equation of motion of a nanorod without inertia of the lateral motion ($r_g=0$ or $\nu=0$) was obtained by Gul et al. [13]. Also, neglecting the inertia of lateral motion and the scale parameter ($\eta=0$) in Eq. (28) yields the natural frequencies for the classical rod theory. According to Eq. (28), maximum mode number (n) can be obtained by $n = 1/\pi\beta$ for a given length of the nanorod. This maximum mode number represents the van Hove singularity. When $n > 1/\pi\beta$, the roots of natural frequencies given in Eq. (28) take imaginary values and there is no vibration above this critical mode number in DM–Love nanorod

Table 2 Natural frequencies (THz) of free–free (5,5) and (5,0) carbon nanotubes for the first three modes

Length (nm)	Mode number	Classical theory	DM theory with Love's assumption (zigzag)	DM theory with Love's assumption (armchair)	MD [19]
$L=24.4$	1st	0.549	0.550	0.550	0.550
	2nd	1.099	1.098	1.098	1.100
	3rd	1.649	1.650	1.650	1.650
$L=5$	1st	2.683	2.678	2.678	–
	2nd	5.365	5.345	5.361	–
	3rd	8.048	7.955	7.971	–

($\nu = 1/3$ and $\eta = 0.246$ nm)

Table 3 Natural frequencies (THz) of a clamped-free (5,5) and (5,0) carbon nanotubes for the first mode

Length (nm)	Mode number	Classical theory	DM theory with Love's assumption (zigzag)	DM theory with Love's assumption (armchair)	MD [19]
$L=12.2$	1st	0.5498	0.5490	0.5490	0.5440

($\nu = 1/3$ and $\eta = 0.246$ nm)

model. Meaningful natural frequencies of the nanorods can be obtained for $L=1$ nm up to $n=7$ mode number and for $L=2$ nm up to $n=15$ in the present DM theory, whereas infinite number of frequency modes can be observed for the classical elasticity model. For the clamped-free (C–F) nanorod model, the classical and the non-classical boundary conditions can be expressed as

$$\text{Free end} \;:\; N = \left[U'(\bar{x})\left(1-\Omega^2 r_g^2 v^2\right)+\beta^2 U'''(\bar{x})\right] = 0 \;\text{(classical)}, \quad U(\bar{x})'' = 0 \;\text{(non}-\text{classical) at } \bar{x}=0,1. \tag{29}$$

It should be pointed out that free boundary conditions depend on both scale parameter and lateral inertia, whereas clamped boundary conditions are independent from these effects. By using the boundary conditions given in Eq. (29) with Eq. (23), the solution can be obtained in matrix form as

$$\begin{bmatrix} 0 & 1 & 0 & 1 \\ 0 & -\gamma^2 & 0 & -\theta^2 \\ Cs(\gamma)\gamma T-\beta^2\gamma^3 Cs(\gamma) & -S(\gamma)\gamma T+\beta^2\gamma^3 S(\gamma) & Cs(\theta)\theta T-\beta^2\theta^3 Cs(\theta) & -S(\theta)\theta T+\beta^2\theta^3 S(\gamma) \\ -\gamma^2 S(\gamma) & -\gamma^2 Cs(\gamma) & -\theta^2 S(\theta) & -\theta^2 Cs(\theta) \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \\ c_3 \\ c_4 \end{bmatrix} = 0 \tag{30}$$

where S: sine, Cs: cosine and $T = \left(1-\Omega^2 r_g^2 v^2\right)$. The determinant of the coefficient matrix in Eq. (30) must be zero, so it leads to the frequency equation as follows

$$Z_1\left[Z_2 - Z_3 - Z_4 + Z_5\right] = 0 \tag{31}$$

where

$$\begin{aligned} Z_1 &= -\gamma\theta\left(\gamma^2-\theta^2\right), \\ Z_2 &= \gamma T \sin(\gamma)\cos(\theta), \\ Z_3 &= \theta T \cos(\gamma)\sin(\theta), \\ Z_4 &= \gamma\beta^2\theta^2 \sin(\gamma)\cos(\theta), \\ Z_5 &= \gamma^2\beta^2\theta \cos(\gamma)\sin(\theta). \end{aligned} \tag{32}$$

Solution of Eq. (31) gives natural frequencies of the DM nanorod model with Love's assumption for the C–F boundary condition. It is noted that neglecting the $r_g=0$ or $\nu=0$ gives the natural frequencies of the DM nanorod model as a special case given in [13].

5 Validation and discussion

In this section, numerical results are presented for the longitudinal vibration of nanorods considering the inertia of lateral motion based on the DM theory. We give a comparison of the natural frequencies obtained by the DM theory with the classical elasticity, the nonlocal theory and the molecular dynamics (MD) solution for validation. Natural frequencies

Table 4 Natural frequencies (THz) of a clamped-free (5,5) and (5,0) carbon nanotubes for the first mode

r_g	Classical theory with Love's assumption [8]	Nonlocal theory with Love's assumption [8]		DM theory with Love's assumption (zigzag)		DM theory with Love's assumption (armchair)	
		$e_0a/L=0.1$	$e_0a/L=0.2$	$L=5$ nm	$L=24.4$ nm	$L=5$ nm	$L=24.4$ nm
0.01	1.5708	1.5518	1.4986	1.5696	1.5705	1.5696	1.5705
0.1	1.5691	1.5501	1.4971	1.5680	1.5689	1.5680	1.5689
0.2	1.5639	1.5451	1.4926	1.5632	1.5642	1.5632	1.5642

($\nu = 1/3$ and $\eta = 0.246$ nm)

Table 5 Dimensionless natural frequencies for C–C nanorods (zigzag model) with $\nu = 1/3$ and $\eta = 0.1421$ nm

L (nm)		Classical theory	Doublet mechanics theory						
			Love				Classical Love		
			$r_g=0$	$r_g=0.01$	$r_g=0.05$	$r_g=0.1$	$r_g=0.01$	$r_g=0.05$	$r_g=0.1$
1	1st	3.1420	3.1153	3.1152	3.1119	3.1016	3.1414	3.1381	3.1277
	2nd	6.2830	6.0709	6.0698	6.0441	5.9658	6.2820	6.2554	6.1744
	3rd	9.4250	8.6919	8.6884	8.6063	8.3640	9.4210	9.3319	9.0692
	4th	12.566	10.768	10.760	10.581	10.075	12.557	12.348	11.758
2	1st	3.1420	3.1350	3.1349	3.1315	3.1212	3.1414	3.1381	3.1277
	2nd	6.2830	6.2307	6.2296	6.2033	6.1229	6.2820	6.2554	6.1744
	3rd	9.4250	9.2470	9.2433	9.1559	8.8981	9.4210	9.3319	9.0692
	4th	12.566	12.141	12.133	11.931	11.361	12.557	12.348	11.758
3	1st	3.1420	3.1386	3.1385	3.1352	3.1248	3.1414	3.1381	3.1277
	2nd	6.2830	6.2599	6.2588	6.2323	6.1516	6.2820	6.2554	6.1744
	3rd	9.4250	9.3461	9.3424	9.2541	8.9936	9.4210	9.3319	9.0692
	4th	12.566	12.379	12.370	12.165	11.583	12.557	12.348	11.758
5	1st	3.1420	3.1405	3.1404	3.1370	3.1266	3.1414	3.1381	3.1277
	2nd	6.2830	6.2748	6.2737	6.2471	6.1662	6.2820	6.2554	6.1744
	3rd	9.4250	9.3965	9.3928	9.3040	9.0420	9.4210	9.3319	9.0692
	4th	12.566	12.499	12.490	12.283	11.695	12.557	12.348	11.758

($\Omega = n\pi$ for C–C nanorods in the classical elasticity theory)

of a free–free single-walled zigzag (5,0) and armchair (5,5) carbon nanotubes are presented for the DM theory under the Love's assumption, and they are compared with the classical elasticity model and MD [19] in Table 2. The length of the carbon nanotube and its thickness are $L=24.4$ nm and $t=0.08$ nm, and material properties of this nanotube are $E=6.85$ TPa, $\nu=0.3$ and $\rho=9517$ kg/m^3 [19] in this table. The DM results are in excellent agreement with the MD solution. The first and third natural frequencies are exactly same for the DM and the MD solution. Also, the classical results agree well with the MD solution for the rod length of 24.4 nm. When the beam length is 5 nm, the difference between the DM and the classical results increases, and it is more apparent for the third mode of vibration. Another remarkable observation can be seen that when $L=5$ nm, frequency results for armchair model (5,5) are higher than zigzag model (5,0) in DM for the second and third vibration modes.

Similarly, the validation of the present DM model is shown in Table 3 for the single-walled zigzag (5,0) and armchair (5,5) carbon nanotubes with C–FC–FC–F boundary conditions. The best agreement can be observed from Table 3 between the DM and MD solutions.

Table 4 presents the natural frequencies obtained for the zigzag (5,0) and armchair (5,5) carbon nanotubes with C–F boundary conditions. It is seen that DM predicts lower frequencies than classical Love assumption for both zigzag (5,0) and armchair (5,5) models, whereas it gives higher frequencies than nonlocal models for the considered r_g values. We believe that the difference between DM and nonlocal theory is due to unclear nature of the scale parameters used in nonlocal models.

In Tables 5 and 6, the first four modes of vibration frequencies are shown for the DM theory for zigzag model under the Love's assumption, classical Love theory and classical elasticity theory for the C–F and C–C boundary conditions. The results are given for the different radii of the

Table 6 Dimensionless natural frequencies for C–F nanorods (zigzag model) with $\nu = 1/3$ and $\eta = 0.1421$ nm

L (nm)		Classical theory	Doublet mechanics theory						
			Love				Classical Love		
			$r_g=0$	$r_g=0.01$	$r_g=0.05$	$r_g=0.1$	$r_g=0.01$	$r_g=0.05$	$r_g=0.1$
1	1st	1.5710	1.5684	1.5684	1.5674	1.5669	1.5705	1.5689	1.5673
	2nd	4.7120	4.6295	4.6295	4.6154	4.5823	4.7106	4.6917	4.6619
	3rd	7.8540	7.4220	7.4175	7.3630	7.1832	7.8464	7.7793	7.1639
	4th	10.996	9.3280	9.3100	8.9466	7.8903	10.988	10.782	10.379
2	1st	1.5710	1.5710	1.5700	1.5700	1.5684	1.5705	1.5689	1.5673
	2nd	4.7120	4.6906	4.6906	4.6806	4.6436	4.7106	4.6917	4.6619
	3rd	7.8540	7.7532	7.7532	7.6958	7.5593	7.8464	7.7793	7.1639
	4th	10.996	10.692	10.679	10.616	10.176	10.988	10.782	10.379
3	1st	1.5710	1.5710	1.5705	1.5700	1.5689	1.5705	1.5689	1.5673
	2nd	4.7120	4.7053	4.7040	4.6906	4.6436	4.7106	4.6917	4.6619
	3rd	7.8540	7.8122	7.8065	7.7840	7.6050	7.8464	7.7793	7.1639
	4th	10.996	10.813	10.744	10.729	10.339	10.988	10.782	10.379
5	1st	1.5710	1.5710	1.5705	1.5705	1.5689	1.5705	1.5689	1.5673
	2nd	4.7120	4.7120	4.7088	4.6992	4.6671	4.7106	4.6917	4.6619
	3rd	7.8540	7.8322	7.8086	7.7867	7.6362	7.8464	7.7793	7.1639
	4th	10.996	10.952	10.945	10.813	10.407	10.988	10.782	10.379

($\Omega = (2n-1)\pi/2$ for C–F nanorods in the classical elasticity theory)

gyration (r_g) and different rod lengths. It is seen that natural frequencies predicted by DM are less than the classical elasticity solution for both the boundary conditions. This is due to strain gradient effect of the DM theory and increasing kinetic energy by including lateral inertia in the formulation of Love theory. The decrease in the dimensionless frequency is more prominent for the low nanorod lengths, since the scale effects become more important for the short nanorods. This effect is more pronounced for higher modes of the vibration. Increase in the radius of the gyration decreases the natural frequencies since the rod becomes more thinner. The difference between the DM theory and the classical elasticity model increases with the increase in the mode number. For the higher modes of vibration, wavelengths decrease and approach to the intrinsic length scale of the nanorods. The difference between the DM and the classical theory is 15.17% and 16.7% for the fourth mode of the C–F and C–C nanorods with length $L=1$ nm, respectively. The small-scale effects are lost approximately with the increase in the nanorod length. The differences between the DM results and the classical nanorod results are 0.4% and 0.53% for the fourth mode of the C–F and C–C nanorods with length $L=5$ nm, respectively. When the internal length scale is comparable to the length of the nanorod, scale effects are more effective. Considering the rotary inertia of the nanorod in the formulation decreases the non-dimensional frequencies. Decrease in the non-dimensional frequency with respect to the classical elasticity are 24.72% and 28.23% for the fourth mode of the C–F and C–C nanorods with length $L=1$ nm, respectively. Differences between the DM results and classical nanorod results are 6.93% and 5.36% for the fourth mode of the C–F and C–C nanorod with length $L=5$ nm, respectively. Effect of the DM is higher than that

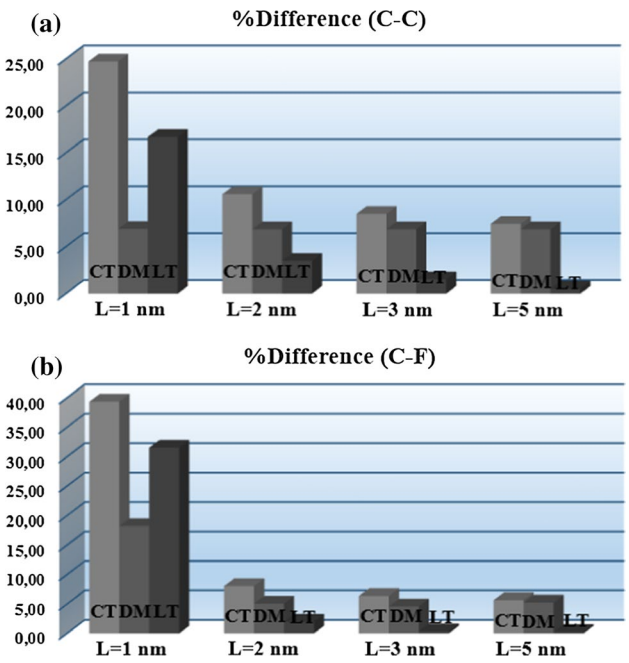

Fig. 3 The percentage difference of theories with respect to DM–Love model for the fourth mode at $r_g=0.1$ (*CT* classical theory, *DM* doublet mechanics, *LT* Love theory)

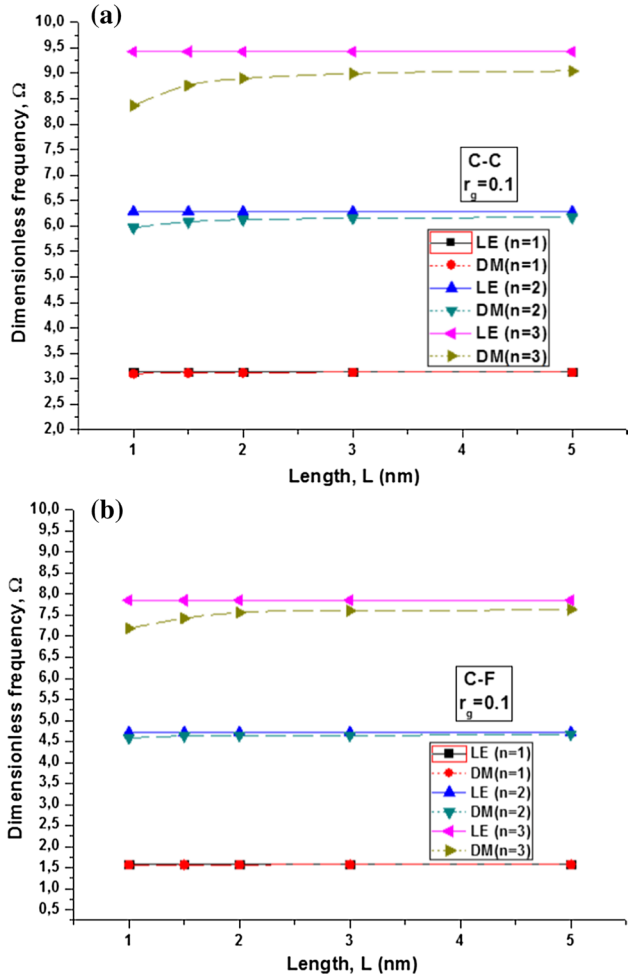

Fig. 4 Variation of dimensionless frequency with length for the first three modes (LE: classical elasticity theory)

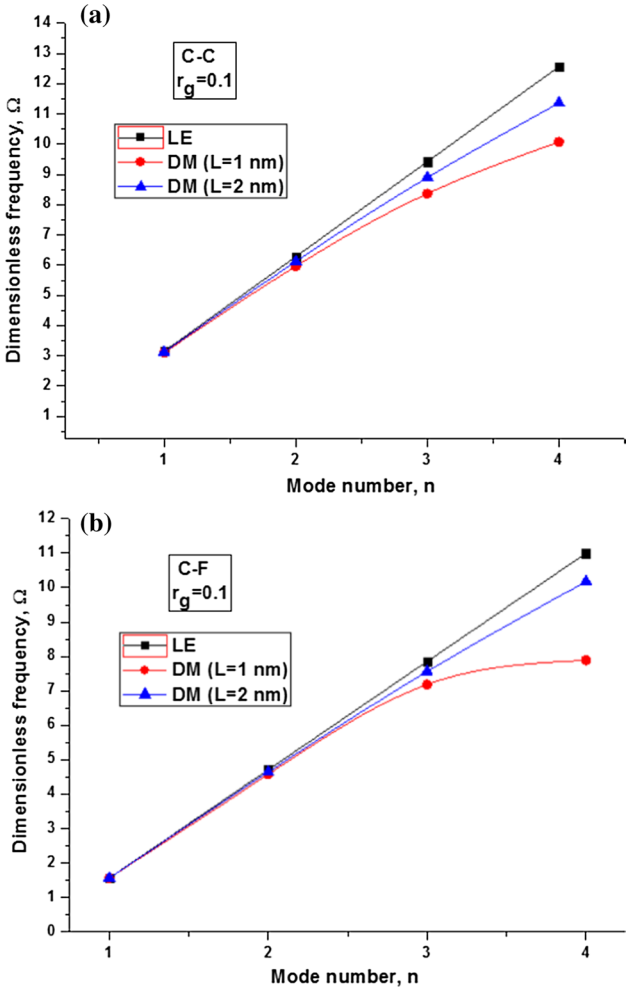

Fig. 5 Variation of dimensionless frequency with mode number (LE: classical elasticity theory)

of lateral inertia for the short nanorods, whereas reverse is true for the longer nanorods.

In Fig. 3, the percentage difference of the dimensionless frequency parameters with respect to the DM–Love rod theory for zigzag model has been shown. It is seen that scale effects are more pronounced especially for short nanorods, whereas lateral inertia is effective in short and moderate lengths. It should be noted that both scale and lateral inertia effects are more apparent for short C–F nanorods when compared to that of C–C nanorods.

In Figs. 4, 5, 6 and 7, the comparison of the natural frequencies obtained by the DM for zigzag model and the classical elasticity theories is shown. $r_g = 0.1$ and $\nu = 0.3$ are considered in these computations. Figure 4 shows the variation of the natural frequencies with the different rod lengths for the first three modes of vibration. It can be seen that DM results are less than the classical elasticity results for the first three modes. The difference between both theories increases with the decrease in the rod length. This is more apparent in C–C condition with respect to the C–F boundary condition.

In Fig. 5, the natural frequencies are given for the first four modes. $L = 1$ nm and $L = 2$ nm are taken into account in the computations. The difference between both theories is more apparent for the higher modes of vibration and for the short nanorods. There is a small difference between the DM and classical elasticity theories for the lower mode numbers.

Figures 6 and 7 show the natural frequencies with the different doublet separation distance for $L = 1$ nm and $L = 2$ nm. It is clearly seen that natural frequencies of the DM theory decrease with the increase in the doublet separation distance (η) especially for the higher modes, since the nodes in the solid are located closely with the decrease in the doublet distance. In this case, solid becomes more homogeneous. It is also seen that decrease in the natural frequencies with the increase in the doublet distance is more prominent for $L = 1$ nm compared to $L = 2$ nm.

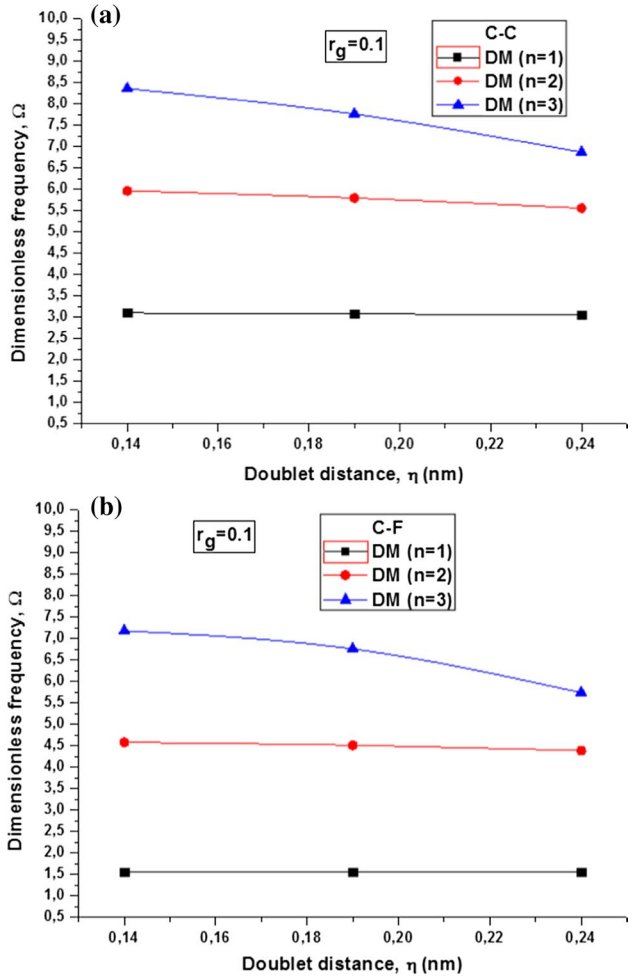

Fig. 6 Variation of dimensionless frequency with doublet distance ($L=1$ nm)

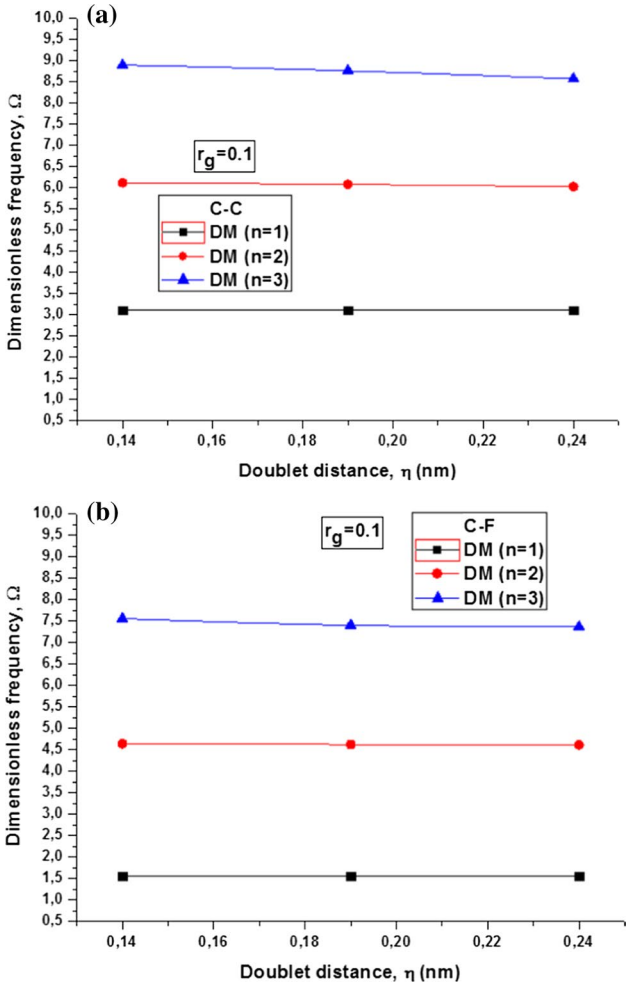

Fig. 7 Variation of dimensionless frequency with doublet distance ($L=2$ nm)

6 Conclusions

A scale-dependent DM theory is modeled for the longitudinal vibration of nanorod considering the lateral inertia effects based on the Love's assumption. Hamilton principle has been extended incorporating the lateral and scale effect for the vibration analysis. The exact vibration frequency equations have been obtained for C–C and C–F boundary conditions. The following remarkable conclusions are drawn:

- Natural frequencies obtained by DM are in an excellent agreement with the MD simulation.
- The inertia of lateral motion decreases the natural frequencies.
- The internal length scale in the present DM model decreases the natural frequencies especially for the short nanorods.
- It is also notable that neglecting the radius of gyration (r_g) or Poisson's ratio (ν) with the scale parameter of the DM model reduces the classical elasticity theory.

Funding The author received no financial support for the research, authorship, and/or publication of this article.

Compliance with ethical standards

Conflict of interest The authors declare that they have no conflict of interest.

Appendix: micro-/macro-stress relations in DM

Under plane stress condition, micro- and macro-stress relations can be defined as

$$\{\sigma\} = [H]\{p\} \tag{33}$$

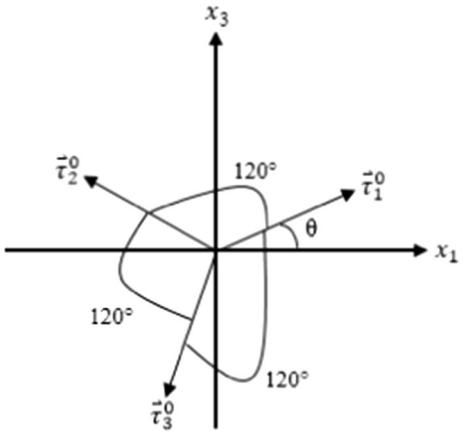

Fig. 8 Three doublets formed in a nanotube

Here, $[H]$ represents the transformation matrix which includes the cosines of the angles $\vec{\tau}_{ij}^{\,0}$ between the micro-stresses and Cartesian coordinates in the considered nano-structure, $\{\sigma\}$ and $\{p\}$ represent the macro- and micro-stress tensor, respectively. Explicit form of $\{\sigma\}$, $\{p\}$ and $[H]$ can be written as

$$\{\sigma\}=\begin{bmatrix}\sigma_{xx}\\ \sigma_{yy}\\ \sigma_{xy}\end{bmatrix},\{p\}=\begin{bmatrix}p_1\\ p_2\\ p_3\end{bmatrix},[H]=\begin{bmatrix}\left(\tau_{11}^o\right)^2 & \left(\tau_{21}^o\right)^2 & \left(\tau_{31}^o\right)^2\\ \left(\tau_{12}^o\right)^2 & \left(\tau_{22}^o\right)^2 & \left(\tau_{32}^o\right)^2\\ \tau_{11}^o\tau_{12}^o & \tau_{21}^o\tau_{22}^o & \tau_{31}^o\tau_{32}^o\end{bmatrix}. \tag{34}$$

where superscript ^{o} represents the initial configuration of the nodes (atoms) in a solid and subscripts "$_{1,2,3}$" represent the direction with respect to three-dimensional Cartesian coordinates. It is clearly seen that extensional macro-stress σ_{xx} is changing with cosines of the angles $\vec{\tau}_{ij}^{\,0}$ of the points (atoms, nodes) in the considered nanostructure. For the present study, we consider the zigzag and armchair nanotube models in the calculations. According to the nanotube model, unit vectors take different values in $[H]$ transformation matrix. Three doublets in a nanotube can be shown in Fig. 8.

It is assumed that nanotube shown in Fig. 8 consists of three doublets with same length and angles between them. Also, the distance between the points (atoms) is same and equals $\eta_\alpha=\eta$, $\alpha=1,2,3$. According to Fig. 8, the unit vectors can be written as

$$\begin{aligned}&\tau_{11}^o=\cos\theta,\quad \tau_{12}^o=\cos 90,\quad \tau_{13}^o=\sin\theta,\\ &\tau_{21}^o=-\sin(30-\theta),\quad \tau_{22}^o=\cos 90,\quad \tau_{23}^o=-\cos(30-\theta),\\ &\tau_{31}^o=-\cos(60-\theta),\quad \tau_{32}^o=\cos 90,\quad \tau_{33}^o=\sin(60-\theta).\end{aligned} \tag{35}$$

In Fig. 8, θ takes from 0° to 30° and this changes the extensional macro-stress σ_{xx} in DM theory. As is seen Sect. 2, when $\theta=0°$ stress expression becomes as Eq. (8) for zigzag nanotube model. In this case, unit vectors in Cartesian coordinates become as follows:

$$\begin{aligned}&\tau_{11}^o=1,\quad \tau_{12}^o=0,\quad \tau_{13}^o=0,\\ &\tau_{21}^o=-1/2,\quad \tau_{22}^o=0,\quad \tau_{23}^o=-\sqrt{3}/2,\\ &\tau_{31}^o=-1/2,\quad \tau_{32}^o=0,\quad \tau_{33}^o=\sqrt{3}/2.\end{aligned} \tag{36}$$

Moreover, same procedure can be applied for obtaining of extensional stress expression in armchair nanotube model in DM. When $\theta=30°$, unit vectors in Cartesian coordinates can be found for armchair nanotube model:

$$\begin{aligned}&\tau_{11}^o=\sqrt{3}/2,\quad \tau_{12}^o=0,\quad \tau_{13}^o=1/2,\\ &\tau_{21}^o=0,\quad \tau_{22}^o=0,\quad \tau_{23}^o=-1,\\ &\tau_{31}^o=-\sqrt{3}/2,\quad \tau_{32}^o=0,\quad \tau_{33}^o=1/2.\end{aligned} \tag{37}$$

Then, applying the plane stress condition obtained before papers [14, 17] and with use of Eqs. (1–7) and by taking $\theta=30°$ extensional macro-stress expression can be obtained as

$$\sigma_{xx}^M=E\left(\varepsilon_{11}+\frac{3}{4}\frac{\eta^2}{12}\frac{\partial^2\varepsilon_{11}}{\partial x^2}\right) \tag{38}$$

It is seen from Eq. (38) that the first term of stress equation called as classical Cauchy stress is same with Eq. (8) whereas the second terms of Eqs. (8, 38) which are called as doublet stresses are different. This difference does not substantially affect the frequency results in zigzag and armchair nanotube models (Tables 2, 3, 4). In this context, armchair nanotube model gives a little bit more frequency results than zigzag model for only higher modes ($n=2,3$) in DM theory.

References

1. Bernoulli D (1753) Reflexions et eclaircissemens sur les nouvelles vibrations des cordes. Hist Mem Acad R Sci Lett Berlin 9:147–172
2. Rayleigh JWS (1945) Theory of sound. Dover Publications, New York
3. Love AEH (2009) A treatise on the mathematical theory of elasticity. Cambridge University Press, Cambridge
4. Aydogdu M (2009) Axial vibration of the nanorods with the nonlocal continuum rod model. Physica E 41(5):861–864
5. Han JB, Hong SY, Song JH et al (2014) Vibrational energy flow models for the Rayleigh-Love and Rayleigh-Bishop rods. J Sound Vib 333:520–540
6. Narendar S (2011) Terahertz wave propagation in uniform nanorods: a nonlocal continuum mechanics formulation including the effect of lateral inertia. Physica E 43:1015–1020
7. Guven U (2011) The investigation of the nonlocal longitudinal stress waves with modified couple stress theory. Acta Mech 221:321–325

8. Li XF, Tang GJ, Shen ZB, Lee KY (2017) Size-dependent resonance frequencies of longitudinal vibration of a nonlocal Love nanobar with a tip nanoparticle. Math Mech Sol 22(6):1529–1542
9. Li XF, Shen ZB, Lee KY (2017) Axial wave propagation and vibration of nonlocal nanorods with radial deformation and inertia. ZAMM-Z Angew Math Mech 97(5):602–616
10. Granik VT (1978) Microstructural mechanics of granular media. Technique report IM/MGU. Moscow State University of Mechanical Engineering, pp 78–241. https://www.researchgate.net/institution/Moscow_State_University_of_Mechanical_Engineering
11. Ferrari M, Granik VT, Imam A, Nadeau JC (1997) Advances in doublet mechanics. Springer, Berlin
12. Kojic M, Vlastelica I, Decuzzi P, Granik VT, Ferrari M (2011) A finite element formulation for the doublet mechanics modeling of microstructural materials. Comput Methods Appl Mech Eng 200:1446–1454
13. Gul U, Aydogdu M, Gaygusuzoglu G (2017) Axial dynamics of a nanorod embedded in an elastic medium using doublet mechanics. Compos Struct 160:1268–1278
14. Gul U, Aydogdu M (2018) Structural modelling of nanorods and nanobeams using doublet mechanics theory. Int J Mech Mater Design 14(2):195–212
15. Vajari AF, Imam A (2016) Torsional vibration of single-walled carbon nanotubes using doublet mechanics. J Appl Math Phys/ZAMP 67:81
16. Vajari AF, Imam A (2016) Axial vibration of single-walled carbon nanotubes using doublet mechanics. Indian J Phys 90(4):447–455
17. Gul U, Aydogdu M, Gaygusuzoglu G (2018) Vibration and buckling analysis of nanotubes (nanofibers) embedded in an elastic medium using Doublet Mechanics. J Eng Math 109(1):85–111
18. Askes H, Suiker ASJ, Sluys LJ (2002) A classification of higher-order strain gradient models—linear analysis. Arch Appl Mech 72:171–188
19. Cao G, Chen X, Kysar JW (2006) Thermal vibration and apparent thermal contraction of single-walled carbon nanotubes. J Mech Phys Solids 54:1206–1236

Publisher's Note Springer Nature remains neutral with regard to jurisdictional claims in published maps and institutional affiliations.