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The nano scale bending and dynamic properties of isolated protein microtubules based on modified strain gradient theory

Djazia Leila Benmansour [1], Abdelhakim Kaci [2,3], Abdelmoumen Anis Bousahla [1,4], Houari Heireche [1], Abdelouahed Tounsi*[3,5], Afaf S. Alwabli [6], Alawiah M. Alhebshi [6], Khalid Al-ghmady [6] and S.R. Mahmoud [7]

[1] *Laboratoire de Modélisation et Simulation Multi-échelle, Département de Physique, Faculté des Sciences Exactes, Département de Physique, Université de Sidi Bel Abbés, Algeria*
[2] *Université Dr Tahar Moulay, Faculté de Technologie, Département de Génie Civil et Hydraulique, BP 138 Cité En-Nasr 20000 Saida, Algérie*
[3] *Material and Hydrology Laboratory, University of Sidi Bel Abbes, Faculty of Technology, Civil Engineering Department, Algeria*
[4] *Centre Universitaire de Relizane, Algérie*
[5] *Department of Civil and Environmental Engineering, King Fahd University of Petroleum & Minerals, 31261 Dhahran, Eastern Province, Saudi Arabia*
[6] *Department of Biology, Faculty of Sciences, King Abdulaziz University, Jeddah, Saudi Arabia*
[7] *GRC Department, Jeddah Community College, King Abdulaziz University, Jeddah, Saudi Arabia*

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Abstract. In this investigation, dynamic and bending behaviors of isolated protein microtubules are analyzed. Microtubules (MTs) can be considered as bio-composite structures that are elements of the cytoskeleton in eukaryotic cells and posses considerable roles in cellular activities. They have higher mechanical characteristics such as superior flexibility and stiffness. In the modeling purpose of microtubules according to a hollow beam element, a novel single variable sinusoidal beam model is proposed with the conjunction of modified strain gradient theory. The advantage of this model is found in its new displacement field involving only one unknown as the Euler-Bernoulli beam theory, which is even less than the Timoshenko beam theory. The equations of motion are constructed by considering Hamilton's principle. The obtained results are validated by comparing them with those given based on higher shear deformation beam theory containing a higher number of variables. A parametric investigation is established to examine the impacts of shear deformation, length scale coefficient, aspect ratio and shear modulus ratio on dynamic and bending behaviors of microtubules. It is remarked that when length scale coefficients are almost identical of the outer diameter of MTs, microstructure-dependent behavior becomes more important.

Keywords: protein microtubules; modified strain gradient theory; single variable beam theory; bending; vibration

1. Introduction

Microtubules (MT) are one of the essential elements that make up the cytoskeleton in eukaryotic cells. They play a major role in several biological processes, such as cell division, intracellular transport, cell motility, movement of the motor proteins and the formation of the mobile nuclei of the flagella and the eyelashes (Scholey *et al*. 2003, Schliwa and Woehlke 2003, Carter and Cross 2005). MTs are made up of both α-tubulin and β-tubulin (see Fig. 1).

They are about one hundred times stiffer than other filaments and are also very flexible. These properties are due to their composite structure and the molecular shuttle considered also as anisotropic structure. Microtubules possess a hollow cylindrical structure and generally come from 13 parallel protofilaments in vivo but this number can vary in a range of 9 to 16 in vitro (Chretien and Wade 1991). Generally, MTs are found with inner and outer diameters about 15 nm and 25 nm, respectively and a length in a range from 10 nm to a 100 μm (Amos and Amos 1991, Howard and Hyman 2003).

After knowing that the above-indicated functions of the microtubules are depending to their mechanical characteristics, the mechanical behavior of MTs has become a topic of an essential interest in many theoretical and experimental investigations (Venier *et al*. 1994, Gittes *et al*. 1993, Kurachi *et al*. 1995, Felgner *et al*. 1996, Vinckier *et al*. 1996, Kis *et al*. 2002, Kikumoto *et al*. 2006, Akgöz and Civalek 2014a). Thus, mathematical models have been

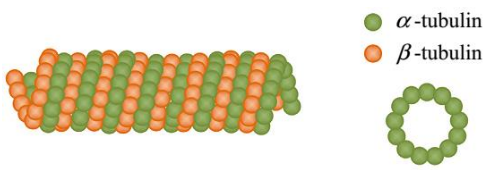

Fig. 1 Structure of a typical microtubule (Akgöz and Civalek 2014a)

*Corresponding author, Ph.D., Professor,
E-mail: tou_abdel@yahoo.com

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widely employed to examine the elastic characteristics and mechanical responses of MTs in recent years. The experimental observations indicated that the bonds between adjacent protofilaments in the longitudinal direction are stronger than those in the transversal direction within protofilaments (Nogales *et al*. 1999, Van-Buren *et al*. 2002, Needleman *et al*. 2004). In addition, the longitudinal Young's modulus of MTs is much higher than the circumferential and shear modulus (Pampaloni *et al*. 2006, Tuszynski *et al*. 2005, Portet *et al*. 2005). These primary remarks as well as the presence of two tubulins demonstrate that MTs have heterogeneous structure and anisotropic characteristics. Consequently, transverse shear influences become more considerable on mechanical behaviors of MTs, especially for short microtubules. Kis *et al*. (2002) examined anisotropic characteristics of single microtubules and they observed that the magnitude of shear modulus is two orders lower than of Young's modulus. Using a finite element method, Kasas *et al*. (2004) investigated the mechanical characteristics of MTs. An orthotropic elastic shell model for MTs is introduced by Li *et al*. (2006) and Wang *et al*. (2006) and they seen that length dependence of flexural rigidity is depending to anisotropic elastic characteristics of MTs. Ghavanloo *et al*. (2010) and Daneshmand and Amabili (2012) are proposed a Euler–Bernoulli beam theory and an orthotropic elastic shell theory incorporating the influences of the viscous cytosol and surrounding filaments to evaluate the coupled oscillations of a single MT embedded in cytoplasm, respectively. Shi *et al*. (2008) and Tounsi *et al*. (2010) developed first and parabolic shear deformation beam theories respectively to consider the impacts of transverse shearing deformation on mechanical characteristics of MTs. Akgöz and Civalek (2014a) presented a microstructure-dependent shear deformation beam theory for bending and vibration investigation of MTs on the basis of modified strain gradient elasticity theory. In addition, atomistic continuum approaches for mechanical investigations of MTs can be found in literature reviews (Xiang and Liew 2011, 2012a, b, 2013).

It should be noted that some experimental investigations have been shown that existing size influences plays a considerable role on mechanic responses of small-scale structures (Poole *et al*. 1996, Lam *et al*. 2003, McFarland and Colton 2005). The classical (conventional) continuum models have no material length size coefficients and fail to evaluate the scale dependent responses of micro- and nano-sized structures. Thus, many non- conventional (higher-order) continuum models have been developed to study the mechanical responses of small-scaled structures such as couple stress model (Mindlin and Tiersten 1962, Koiter 1964, Toupin 1964, Akbaş 2018), micropolar model (Eringen 1967), nonlocal elasticity model (Eringen 1972, 1983, Belkorissat *et al*. 2015, Zemri *et al*. 2015, Larbi Chaht *et al*. 2015, Eltaher *et al*. 2016, Bounouara *et al*. 2016, Ahouel *et al*. 2016, Elmerabet *et al*. 2017, Khetir *et al*. 2017, Bellifa *et al*. 2017a, Bouafia *et al*. 2017, Besseghier *et al*. 2017, Jandaghian and Rahmani 2017, Mouffoki *et al*. 2017, Bouadi *et al*. 2018, Mokhtar *et al*. 2018, Yazid *et al*. 2018) and strain gradient models (Fleck and Hutchinson 1993, Vardoulakis and Sulem 1995, Aifantis 1999, Karami *et al*. 2017, 2018a, b, c, d, e, 2019a, Bensaid *et al*. 2018, Arefi *et al*. 2018).

The theory based on modified strain gradient (Lam *et al*. 2003) is one of the above-indicated higher-order models in which the density of strain energy possesses second-order deformation gradients in addition to first-order deformation gradient. For linear elastic isotropic materials, the mathematical approach and equilibrium equations consider three additional material length scale parameters related to higher-order deformation gradients besides two classical ones. This popular model has been utilized to examine mechanic responses of microbars (Kahrobaiyan *et al*. 2011a, 2013, Narendar *et al*. 2012, Akgöz and Civalek 2013a, 2014b, Güven 2014) and micro-beams (Wang *et al*. 2010, Akgöz and Civalek 2011a, 2012a, 2013b, c, 2014c, Ansari *et al*. 2011, Asghari *et al*. 2012, Artan and Toksöz 2013, Ghayesh *et al*. 2013, Kahrobaiyan *et al*. 2011b, 2012, Zhao *et al*. 2012, Lei *et al*. 2013, Tajalli *et al*. 2013, Al-Basyouni *et al*. 2015).

As indicated above, the diameter and length of microtubules are in the order of nanometers and micrometers, respectively. Thus, modeling and investigation of MTs considering non-conventional continuum models have attracted many scientists recently. The persistence length and stability behaviors of MTs have been studied by Gao and Lei (2009) and Fu and Zhang (2010) by considering the nonlocal elasticity model and modified couple stress model, respectively. Heireche *et al*. (2010) employed a nonlocal Timoshenko beam theory for dynamic of protein microtubules by considering a visco-elastic surrounding cytoplasm. The stability behaviors of MTs in living cells are examined and discussed by Gao and An (2010) by using a nonlocal anisotropic shell model. Shen (2010a, b, c) proposed nonlocal shear deformation shell theories for both linear and nonlinear investigations of MTs. Also, bending and vibration responses of MTs examined based on Euler–Bernoulli beam and non-conventional continuum models (Civalek and Akgöz 2010, Civalek *et al*. 2010, Akgöz and Civalek 2011b, 2012b, Zeverdejani and Beni 2013).

In this article, bending and vibration behaviors of MTs, one of the principal elements of the cytoskeleton in living cells, are examined. In order to model the microtubules such as a hollow cylindrical beam, a single variable shear deformation beam theory is proposed by considering the modified strain gradient elasticity model. This theory is constructed on the basis of the Euler–Bernoulli beam (EBT) including the sinusoidal function in terms of thickness coordinate to consider shear deformation influence and it involves only one equation of motion. The developed model in this study will be attracting the large community of biophysicist investigating in the field of mechanical filament, rather than to the community of engineering.

2. The modified theory of strain gradient elasticity

The modified theory of strain gradient elasticity known generally by MSGT (Lam *et al*. 2003) is one of the widely employed high order continuum models. Contrary to conventional continuum models, this model considers some high order strain gradient with the conventional tensor of strain in the theoretical approaches as vector of dilatation gradient, deviatoric stretch gradient and symmetric tensors of the rotation gradient. The energy of strain U for the modified theory of strain gradient can be expressed by using infinitesimal deformations (Lam *et al*. 2003) as

$$U = \frac{1}{2}\int_0^L \int_A \left(\sigma_{ij}\varepsilon_{ij} + p_i\gamma_i + \tau_{ijk}^{(1)}\eta_{ijk}^{(1)} + m_{ij}^s\chi_{ij}^s\right) dA\ dx \quad (1)$$

in which $\varepsilon_{ij}, \gamma_i, \eta_{ijk}^{(1)}$ and χ_{ij}^s denote the components of the tensor of strain $[\varepsilon]$, the gradient of dilatation vector γ, the tensor of deviatoric stretch gradient $[\eta]^{(1)}$ and the tensor of symmetric rotation gradient χ^s, respectively and are expressed as following

$$\varepsilon_{ij} = \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \quad (2)$$

$$\gamma_i = \frac{\partial \varepsilon_{mm}}{\partial x_i} \quad (3)$$

$$\begin{aligned}\eta_{ijk}^{(1)} &= \frac{1}{3}\left(\frac{\partial \varepsilon_{jk}}{\partial x_i} + \frac{\partial \varepsilon_{ki}}{\partial x_j} + \frac{\partial \varepsilon_{ij}}{\partial x_k}\right) \\ &- \frac{1}{15}\left[\delta_{ij}\left(\frac{\partial \varepsilon_{mm}}{\partial x_k} + 2\frac{\partial \varepsilon_{mk}}{\partial x_m}\right) + \delta_{jk}\left(\frac{\partial \varepsilon_{mm}}{\partial x_i} + 2\frac{\partial \varepsilon_{mi}}{\partial x_m}\right) \right. \\ &\left. + \delta_{ki}\left(\frac{\partial \varepsilon_{mm}}{\partial x_j} + 2\frac{\partial \varepsilon_{mj}}{\partial x_m}\right)\right]\end{aligned} \quad (4)$$

$$\theta_i = \frac{1}{2} e_{ijk}\frac{\partial u_k}{x_j} \quad (5)$$

$$\chi_{ij}^s = \frac{1}{2}\left(\frac{\partial \theta_i}{\partial x_j} + \frac{\partial \theta_j}{\partial x_i}\right) \quad (6)$$

where u_i presents the components of the vector of displacement u and θ_i present the components of the vector of rotation θ, also δ and e_{ijk} are the Kronecker delta and permutation symbols, respectively. In addition, the components of the tensor of Cauchy stress $[\sigma]$ and the tensors of higher-order stress p, $\tau^{(1)}$ and m^s (conjugated with $\varepsilon_{ij}, \gamma_i, \eta_{ijk}^{(1)}$ and χ_{ij}^s respectively) are written as following (Lam *et al*. 2003)

$$\sigma_{ij} = \lambda\delta_{ij}\varepsilon_{mm} + 2G\varepsilon_{ij} \quad (7)$$

$$p_i = 2Gl_0^2\gamma_i \quad (8)$$

$$\tau_{ijk}^{(1)} = 2Gl_1^2\eta_{ijk}^{(1)} \quad (9)$$

$$m_{ij}^s = 2Gl_2^2\chi_{ij}^s \quad (10)$$

where l_0, l_1, l_2 are additional material length size parameters related to gradients of dilatation, gradients of deviatoric stretch and gradients of rotation, respectively. In addition, λ and G are the Lamé constants expressed as

$$\lambda = \frac{E\nu}{(1+\nu)(1-2\nu)} \quad \text{and} \quad G = \frac{E}{2(1+\nu)} \quad (11)$$

3. Formulation of single variable sinusoidal beam theory (SVSBT)

MTs can be considered as a hollow element of beam. Modeling of an isolated microtubule like a simply supported cylindrical hollow element of beam is shown in Fig. 2 in which D_i, D_o and L denote the inner, outer diameters and the length of the MT, respectively.

The displacement field for the present SVSBT can be described by

$$\begin{aligned} u(x,z) &= -z\frac{\partial w}{\partial x} - \beta\, f(z)\frac{\partial^3 w}{\partial x^3} \\ v(x,z) &= 0 \\ w(x,z) &= w(x) \end{aligned} \quad (12)$$

where w are the vertical displacement along the midplane of the beam. β is a coefficient defined in Refs (Zidi *et al*. 2017, Hachemi *et al*. 2017) and is geven by Eq. (31). $f(z)$ is a shape function and is used for determining the transverse shear strain and stress variation within the thickness of the beam (or outer diameter of MTs). $f(z)$ is given by

$$f(z) = \frac{h}{\pi} sin\left(\frac{\pi z}{h}\right) \quad (13)$$

where h presents the height of the beam (D_0). Substituting Eq. (12) in equation (2) gives nonzero deformation components as

$$\left.\begin{aligned} \varepsilon_x &= \frac{\partial u}{\partial x} = -z\frac{\partial^2 w}{\partial x^2} - f(z)\beta\frac{\partial^4 w}{\partial x^4} \\ \varepsilon_{xz} &= \frac{1}{2}\left(\frac{\partial u}{\partial z} + \frac{\partial w}{\partial x}\right) = -\frac{1}{2}f'(z)\beta\frac{\partial^3 w}{\partial x^3} \end{aligned}\right\} \quad (14)$$

where

$$f'(z) = \frac{df}{dz} = cos\left(\frac{\pi z}{h}\right) \quad (15)$$

By using Eq. (14) in Eqs. (3)-(5), the nonzero components of higher-order deformation gradients are

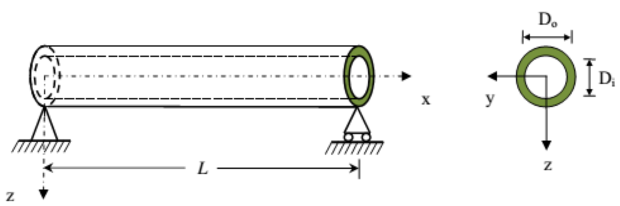

Fig. 2 Continuum modeling of an isolated microtubule as a simply supported cylindrical hollow beam

determined as

$$\gamma_x = \frac{\partial \varepsilon_x}{\partial x} = -z\frac{\partial^3 w}{\partial x^3} - f(z)\beta\frac{\partial^5 w}{\partial x^5}, \tag{16a}$$

$$\gamma_z = \frac{\partial \varepsilon_x}{\partial z} = -\frac{\partial^2 w}{\partial x^2} - f'(z)\beta\frac{\partial^4 w}{\partial x^4} \tag{16b}$$

and

$$\eta_{111}^{(1)} = \frac{1}{5}\left[2\left(-z\frac{\partial^3 w}{\partial x^3} - f(z)\beta\frac{\partial^5 w}{\partial x^5}\right) - \frac{\pi^2}{h^2}f(z)\beta\frac{\partial^3 w}{\partial x^3}\right] \tag{17a}$$

$$\eta_{113}^{(1)} = \eta_{131}^{(1)} = \eta_{311}^{(1)} = -\frac{4}{15}\left(\frac{\partial^2 w}{\partial x^2} + 2f'(z)\beta\frac{\partial^4 w}{\partial x^4}\right) \tag{17b}$$

$$\eta_{122}^{(1)} = \eta_{212}^{(1)} = \eta_{221}^{(1)} = -\frac{1}{5}\left[-z\frac{\partial^3 w}{\partial x^3} - f(z)\beta\frac{\partial^5 w}{\partial x^5} + \frac{\pi^2}{3h^2}f(z)\beta\frac{\partial^3 w}{\partial x^3}\right] \tag{17c}$$

$$\eta_{133}^{(1)} = \eta_{313}^{(1)} = \eta_{331}^{(1)} = -\frac{1}{5}\left(-z\frac{\partial^3 w}{\partial x^3} - f(z)\beta\frac{\partial^5 w}{\partial x^5} - \frac{4}{3}\frac{\pi^2}{h^2}f(z)\beta\frac{\partial^3 w}{\partial x^3}\right) \tag{17d}$$

$$\eta_{223}^{(1)} = \eta_{232}^{(1)} = \eta_{322}^{(1)} = \frac{1}{15}\left(\frac{\partial^2 w}{\partial x^2} + 2f'(z)\beta\frac{\partial^4 w}{\partial x^4}\right) \tag{17e}$$

$$\eta_{333}^{(1)} = \frac{1}{5}\left(\frac{\partial^2 w}{\partial x^2} + 2f'(z)\beta\frac{\partial^4 w}{\partial x^4}\right) \tag{17f}$$

$$\chi_{xy}^s = \frac{1}{2}\left(\frac{\partial \theta_x}{\partial y} + \frac{\partial \theta_y}{\partial x}\right) = -\frac{1}{2}\left[\frac{\partial^2 w}{\partial x^2} + \frac{1}{2}\beta f'(z)\frac{\partial^4 w}{\partial x^4}\right] \tag{18a}$$

$$\chi_{yz}^s = \frac{1}{2}\left(\frac{\partial \theta_y}{\partial z} + \frac{\partial \theta_z}{\partial y}\right) = \frac{\pi^2}{4h^2}\beta f(z)\frac{\partial^3 w}{\partial x^3} \tag{18b}$$

Employing Eq. (14) in Eq. (7), the nonzero components of conventional stress tensor σ can be expressed as

$$\sigma_x = E\eta\left(-z\frac{\partial^2 w}{\partial x^2} - f(z)\beta\frac{\partial^4 w}{\partial x^4}\right), \tag{19a}$$

$$\tau_{xz} = -Gf'(z)\beta\frac{\partial^3 w}{\partial x^3} \tag{19b}$$

$$\sigma_y = \sigma_z = \lambda\left(-z\frac{\partial^2 w}{\partial x^2} - f(z)\beta\frac{\partial^4 w}{\partial x^4}\right) \tag{19c}$$

where

$$\eta = \frac{(1-\nu)}{(1+\nu)(1-2\nu)} \quad \text{and} \quad \lambda = \frac{E\nu}{(1+\nu)(1-2\nu)} \tag{20}$$

Also, substituting Eqs. (16)-(18) in Eqs. (8)-(10) gives the nonzero components of higher order stresses such as

$$p_x = 2Gl_0^2\gamma_x = 2Gl_0^2\left(-z\frac{\partial^3 w}{\partial x^3} - f(z)\beta\frac{\partial^5 w}{\partial x^5}\right) \tag{21a}$$

$$p_z = 2Gl_0^2\gamma_z = -2Gl_0^2\left(\frac{\partial^2 w}{\partial x^2} + f'(z)\beta\frac{\partial^4 w}{\partial x^4}\right) \tag{21b}$$

$$\tau_{111}^{(1)} = 2Gl_1^2\eta_{111}^{(1)} = \frac{2}{5}Gl_1^2\left[2\left(-z\frac{\partial^3 w}{\partial x^3} - f(z)\beta\frac{\partial^5 w}{\partial x^5}\right) - \frac{\pi^2}{h^2}f(z)\beta\frac{\partial^3 w}{\partial x^3}\right] \tag{22a}$$

$$\tau_{113}^{(1)} = \tau_{131}^{(1)} = \tau_{311}^{(1)} = -\frac{8}{15}Gl_1^2\left(\frac{\partial^2 w}{\partial x^2} + 2f'(z)\beta\frac{\partial^4 w}{\partial x^4}\right) \tag{22b}$$

$$\tau_{122}^{(1)} = \tau_{212}^{(1)} = \tau_{221}^{(1)} = -\frac{2}{5}Gl_1^2\left[-z\frac{\partial^3 w}{\partial x^3} - f(z)\beta\frac{\partial^5 w}{\partial x^5} + \frac{\pi^2}{3h^2}f(z)\beta\frac{\partial^3 w}{\partial x^3}\right] \tag{22c}$$

$$\tau_{133}^{(1)} = \tau_{313}^{(1)} = \tau_{331}^{(1)} = -\frac{2}{5}Gl_1^2\left(-z\frac{\partial^3 w}{\partial x^3} - f(z)\beta\frac{\partial^5 w}{\partial x^5} - \frac{4}{3}\frac{\pi^2}{h^2}f(z)\beta\frac{\partial^3 w}{\partial x^3}\right) \tag{22d}$$

$$\tau_{223}^{(1)} = \tau_{232}^{(1)} = \tau_{322}^{(1)} = \frac{2}{15}Gl_1^2\left(\frac{\partial^2 w}{\partial x^2} + 2f'(z)\beta\frac{\partial^4 w}{\partial x^4}\right) \tag{22e}$$

$$\tau_{333}^{(1)} = \frac{2}{5}Gl_1^2\left(\frac{\partial^2 w}{\partial x^2} + 2f'(z)\beta\frac{\partial^4 w}{\partial x^4}\right) \tag{22f}$$

$$m_{xy}^s = 2Gl_2^2\chi_{xy}^s = -Gl_2^2\left[\frac{\partial^2 w}{\partial x^2} + \frac{1}{2}\beta f'(z)\frac{\partial^4 w}{\partial x^4}\right] \tag{23a}$$

$$m_{yz}^s = 2Gl_2^2\chi_{yz}^s = \frac{Gl_2^2\pi^2}{2h^2}\beta f(z)\frac{\partial^3 w}{\partial x^3} \tag{23b}$$

The first variation of the strain energy for the MTs can be written using the above conventional and unconventional (higher order) stress and strain components into equation (1) (by neglecting the Poisson influence) as

$$\begin{aligned}\delta U &= \int_0^L \int_A \left(\sigma_{ij}\delta\varepsilon_{ij} + p_{ij}\delta\gamma_{ij} + \tau_{ijk}^{(1)}\delta\eta_{ijk}^{(1)} + m_{ij}^s\delta\chi_{ij}^s\right) dA dx \\ &= \int_0^L \left[\left(-\frac{6BI}{\pi^2}\beta^2\frac{\partial^{10} w}{\partial x^{10}} + \left(S_4\beta^2 - 4BA\beta\frac{h^2}{\pi^3}\right)\frac{\partial^8 w}{\partial x^8} + (2S_3\beta - S_1\beta^2 - BI)\frac{\partial^6 w}{\partial x^6} + S_2\frac{\partial^4 w}{\partial x^4}\right)\delta w\right] dx\end{aligned} \tag{24}$$

where

$$B = 2G\left(l_0^2 + \frac{2}{5}l_1^2\right), \quad S_1 = GA\left(\frac{1}{2} + \frac{\pi^2}{h^2}\left(\frac{4}{15}l_1^2 + \frac{1}{8}l_2^2\right)\right), \tag{25}$$

$$S_2 = EI + GA\left(2l_0^2 + \frac{8}{15}l_1^2 + l_2^2\right),$$
$$S_3 = \frac{24EI}{\pi^3} + \frac{GA}{\pi}\left(4l_0^2 + \frac{4}{3}l_1^2 + l_2^2\right), \quad (25)$$
$$S_4 = \frac{6EI}{\pi^2} + GA\left(l_0^2 + \frac{2}{3}l_1^2 + \frac{1}{8}l_2^2\right)$$

where A and I are the "*cross-sectional area*" and the "*second moment*" of area, respectively. On the other hand, the variation of "*potential energy*" of the applied loads can be written as (Zidi *et al*. 2014, Bellifa *et al*. 2016, Younsi *et al*. 2018, Meksi *et al*. 2019, Zarga *et al*. 2019)

$$\delta V = \int_A q\delta w dA \quad (26)$$

where q is the distributed transverse load.

The variation of kinetic energy of the beam can be written in the form (Bessaim *et al*. 2013, Meziane *et al*. 2014, Attia *et al*. 2015, Yahia *et al*. 2015, Bourada *et al*. 2015, Bennoun *et al*. 2016, Boukhari *et al*. 2016, Abdelaziz *et al*. 2017, Abualnour *et al*. 2018, Bouhadra *et al*. 2018, Fourn *et al*. 2018, Belabed *et al*. 2018, Yeghnem *et al*. 2017, Zaoui *et al*. 2019, Bourada *et al*. 2019)

$$\delta K = \frac{1}{2}\int_0^L \int_A \rho\left(\left(\frac{\partial u}{\partial t}\right)^2 + \left(\frac{\partial v}{\partial t}\right)^2 + \left(\frac{\partial w}{\partial t}\right)^2\right) dAdx \quad (27)$$

where ρ is the mass density. From Eqs. (12) and (27), the first variation of the kinetic energy can be given as

$$\delta\, K = \int_0^L \left\{\rho A[\dot{w}_0 \delta \dot{w}_0] + \rho I\left(\frac{\partial \dot{w}_0}{\partial x}\frac{\partial \delta\, \dot{w}_0}{\partial x}\right)\right.$$
$$+ \frac{6}{\pi^2}\rho I \beta^2\left(\frac{\partial^3 \dot{w}_0}{\partial x^3}\frac{\partial^3 \delta\, \dot{w}_0}{\partial x^3}\right) \quad (28)$$
$$\left. + \frac{24}{\pi^3}\rho I \beta\left(\frac{\partial \dot{w}_0}{\partial x}\frac{\partial^3 \delta\, \dot{w}_0}{\partial x^3} + \frac{\partial^3 \dot{w}_0}{\partial x^3}\frac{\partial \delta\, \dot{w}_0}{\partial x}\right)\right\} dx$$

Hamilton's principle is used herein to derive the equations of motion. The principle can be stated in analytical form as (Tounsi *et al*. 2013, Belabed *et al*. 2014, Hebali *et al*. 2014, Bousahla *et al*. 2014, Mahi *et al*. 2015, Hamidi *et al*. 2015, Beldjelili *et al*. 2016, Houari *et al*. 2016, Bouderba *et al*. 2016, Bellifa *et al*. 2017b, Ait Atmane *et al*. 2017, Sekkal *et al*. 2017, Menasria *et al*. 2017, Attia *et al*. 2018, Benchohra *et al*. 2018, Tounsi *et al*. 2019, Khiloun *et al*. 2019)

$$0 = \int_0^T (\delta U + \delta V - \delta K)\, dt \quad (29)$$

$$\delta w{:} - \frac{6BI}{\pi^2}\beta^2\frac{\partial^{10} w}{\partial x^{10}} + \left(S_4\beta^2 - 4BA\beta\frac{h^2}{\pi^3}\right)\frac{\partial^8 w}{\partial x^8}$$
$$+ (2S_3\beta - S_1\beta^2 - BI)\frac{\partial^6 w}{\partial x^6} + S_2\frac{\partial^4 w}{\partial x^4} + q \quad (30)$$
$$= \rho A\frac{\partial^2 w}{\partial t^2} - \rho I\frac{\partial^4 w}{\partial x^2 \partial t^2} - \beta\frac{48I}{\pi^3}\frac{\partial^6 w}{\partial x^4 \partial t^2}$$
$$-\beta^2\frac{6I}{\pi^2}\frac{\partial^8 w}{\partial x^6 \partial t^2}$$

and

$$\beta = \frac{S_3\pi^3 + 2\alpha^2 BAh^2}{\pi(S_1\pi^2 + S_4\alpha^2\pi^2 + 6BI\alpha^4)} \quad (31)$$

4. Analytical solutions

In this section, Navier solution procedure is used to determine analytical solutions for bending and dynamic problems of the simply supported MTs. The following expansions of generalized displacements which include undetermined Fourier coefficients and certain trigonometric functions can be successfully employed as

$$w = \sum_{m=1}^{\infty} W_m e^{i\omega_m t} sin(\alpha x) \quad (32)$$

where $\alpha = m\pi/a$ and W_m are arbitrary parameters to be determined; ω_m is eigenfrequency associated with m^{th} eigenmode.

4.1 Bending analysis

The transverse load q is also expanded in the Fourier series as

$$q(x) = \sum_{m=1}^{\infty} q_m\, sin(\alpha x) \quad (33)$$

$$Q_m = \frac{2}{L}\int_0^L q(x)\, sin(\,\alpha x) dx \quad (34)$$

and Q_m can be expressed for point load acted on the midspan of the MTs

$$Q_m = \frac{2Q_0}{L} sin\frac{m\pi}{2} \quad \text{for} \quad m = 1, 2, 3 \quad (35)$$

Substituting Eq. (33) into Eq. (30), the analytical solutions can be obtained from

$$= 2Gl_1^2\eta_{111}^{(1)}$$
$$= \frac{2}{5}Gl_1^2\left[2\left(-z\frac{\partial^3 w}{\partial x^3} - f(z)\beta\frac{\partial^5 w}{\partial x^5}\right) - \frac{\pi^2}{h^2}f(z)\beta\frac{\partial^3 w}{\partial x^3}\right] \quad (36)$$

Solving the above algebraic equation set in Eq. (36), the Fourier coefficient W_m can be determined. Analytical expression of w(x) obtained for the simply supported MTs in bending by substituting this coefficient into Eq. (32).

4.2 Free vibration analysis

Substituting Eq. (32) into Eq. (30) as the equations of motion for free vibration without external applied load, the following equation is determined as

Table 1 Maximum deflections (μm) of the simply supported microtubule under point load (Q_0 = 0.01 nN, $l = D_0$)

r	Beam theory	$L = 50D_0$			$L = 500D_0$		
		CT	MCST	MSGT	CT	MCST	MSGT
Isotropic	EBT	0.0244	0.0044	0.0014	24.3803	4.4128	1.4351
	Akgöz and Civalek (2014a)	0.0244	0.0044	0.0014	24.3806	4.4128	1.4352
	Present	0.0244	0.0044	0.0014	24.3806	4.4128	1.4352
10^{-4}	EBT	0.0244	0.0244	0.0243	24.3803	24.3516	24.2794
	Akgöz and Civalek (2014a)	0.1251	0.0558	0.0372	25.5537	24.6920	24.4148
	Present	0.1251	0.0558	0.0371	25.5536	24.6919	24.4147
10^{-5}	EBT	0.0244	0.0244	0.0244	24.3803	24.3774	24.3702
	Akgöz and Civalek (2014a)	0.6526	0.2778	0.1381	35.7165	27.7240	25.7122
	Present	0.6525	0.2778	0.1381	35.7164	27.7239	25.7121
10^{-6}	EBT	0.0244	0.0244	0.0244	24.3803	24.3800	24.3793
	Akgöz and Civalek (2014a)	1.4478	1.0780	0.7053	125.1389	55.8992	37.3154
	Present	1.4478	1.0780	0.7053	125.1393	55.8992	37.3153

Table 2 Fundamental frequencies (MHz) of the simply supported microtubule ($l = D_0$)

r	Beam theory	$L = 50D_0$			$L = 500D_0$		
		CT	MCST	MSGT	CT	MCST	MSGT
Isotropic	EBT	6.0425	14.2030	24.9082	0.0604	0.1421	0.2491
	Akgöz and Civalek (2014a)	6.0394	14.1998	24.8939	0.0604	0.1421	0.2491
	Present	6.0393	14.1998	24.8938	0.0604	0.1420	0.2491
10^{-4}	EBT	6.0425	6.0461	6.0551	0.604	0.0605	0.0606
	Akgöz and Civalek (2014a)	2.7594	4.1341	5.0151	0.0593	0.0601	0.0604
	Present	2.7593	4.1341	5.0150	0.0592	0.0601	0.0604
10^{-5}	EBT	6.0425	6.0429	6.0438	0.0604	0.0604	0.0604
	Akgöz and Civalek (2014a)	1.1788	1.8302	2.6228	0.0511	0.0572	0.0591
	Present	1.1787	1.8302	2.6227	0.0510	0.0572	0.0591
10^{-6}	EBT	6.0425	6.0426	6.0426	0.0604	0.0604	0.0604
	Akgöz and Civalek (2014a)	0.7851	0.9121	1.1327	0.0276	0.0413	0.0501
	Present	0.7851	0.9120	1.1327	0.0275	0.0413	0.0500

$$(K - \omega^2 M)W_m = 0 \tag{37}$$

where

$$K = \alpha^4 \left[\frac{6BI}{\pi^2}\beta^2\alpha^6 + \left(S_4\beta^2 - 4BA\beta\frac{h^2}{\pi^3} \right)\alpha^4 + (S_1\beta^2 + BI - 2S_3\beta)\alpha^2 + S_2 \right] \tag{38a}$$

$$M = \rho A + \rho I \alpha^2 - \frac{48I}{\pi^3}\rho\beta\alpha^4 + \frac{6I}{\pi^2}\rho\beta^2\alpha^6 \tag{38b}$$

5. Results and discussion

In order to demonstrate the influences of material length scale parameters and shear deformation, some numerical examples are presented on flexural and dynamics responses microtubules.

For illustrative purposes, a simply supported MT is taken as an example with the following material and geometric properties (Heireche *et al.* 2010): Young's modulus E = 1GPa, Poisson ratio $\nu = 0.3$, mass density per unit volume ρ = 1470 kg/m^3, shear modulus ratio $r = G/E$ varying between 10^{-6} and 10^{-4}, inner radius r_i= 7.5 nm, outer radius r_o= 12.5 nm and the length of MT L varying between 1.25 μm and 12.5 μm. All material length scale parameters are considered to be equal to each other as $l_0 = l_1 = l_2$. If two parameters of length scale (l_0 and l_1) or all of them are zero, the proposed model will be transformed modified couple stress (MCST) and classical models (CT), respectively. The results obtained by the present single variable sinusoidal beam model are compared with those obtained by Akgöz and Civalek (2014a) and Euler beam theory (EBT). In addition, it should be noted that the solid lines, the dotted lines, and the dashed lines of

Table 3 Second natural frequencies (MHz) of the simply supported microtubule ($l = D_0$)

R	Beam theory	$L = 50D_0$			$L = 500D_0$		
		CT	MCST	MSGT	CT	MCST	MSGT
Isotropic	EBT	24.1579	56.7834	99.6201	0.2417	0.5682	0.9964
	Akgöz and Civalek (2014a)	24.1077	56.7330	99.3923	0.2417	0.5682	0.9963
	Present	24.1077	56.7329	99.3922	0.2417	0.5682	0.9963
10^{-4}	EBT	24.1579	24.1721	24.2081	0.2417	0.2419	0.2422
	Akgöz and Civalek (2014a)	6.4580	10.4734	14.4957	0.2244	0.2365	0.2400
	Present	6.4579	10.4734	14.4957	0.2244	0.2365	0.2400
10^{-5}	EBT	24.1579	24.1593	24.1629	0.2417	0.2418	0.2418
	Akgöz and Civalek (2014a)	3.4584	4.5236	6.1472	0.1508	0.2000	0.2222
	Present	3.4584	4.5235	6.1472	0.1507	0.2000	0.2222
10^{-6}	EBT	24.1579	24.1581	24.1584	0.2417	0.2417	0.2417
	Akgöz and Civalek (2014a)	2.9675	3.1108	3.3952	0.0646	0.1046	0.1446
	Present	2.9675	3.1108	3.3951	0.0646	0.1046	0.1446

Table 4 Thirs natural frequencies (MHz) of the simply supported microtubule ($l = D_0$)

R	Beam theory	$L = 50D_0$			$L = 500D_0$		
		CT	MCST	MSGT	CT	MCST	MSGT
Isotropic	EBT	54.3098	127.6557	224.0976	0.5439	1.2785	2.2418
	Akgöz and Civalek (2014a)	54.0576	127.4031	222.9556	0.5439	1.2784	2.2417
	Present	54.0576	127.4031	222.9555	0.5439	1.2784	2.2417
10^{-4}	EBT	54.3098	54.3418	54.4228	0.5439	0.5442	0.5450
	Akgöz and Civalek (2014a)	10.9585	17.1998	24.6428	0.4664	0.5179	0.5341
	Present	10.9585	17.1998	24.6428	0.4664	0.5179	0.5341
10^{-5}	EBT	54.3098	54.3130	54.3211	0.5439	0.5439	0.5440
	Akgöz and Civalek (2014a)	7.1213	8.3789	10.5337	0.2582	0.3820	0.4578
	Present	7.1213	8.3789	10.5337	0.2582	0.3820	0.4578
10^{-6}	EBT	54.3098	54.3101	543109	0.5439	0.5439	0.5439
	Akgöz and Civalek (2014a)	6.6021	6.7497	7.0538	0.1096	0.1716	0.2455
	Present	6.6021	6.7497	7.0537	0.1096	0.1716	0.2455

the figures indicate the results for CT, MCST, and MSGT, respectively.

Comparisons of maximum deflections under point load acted on the midspan of the MT, first, second and third natural frequencies with different shear modulus ratio and geometric ratio corresponding to various beam theories and models are presented in Tables 1–4, respectively.

It is seen that the results obtained by the present single variable sinusoidal theory are in excellent agreement with those obtained by Akgöz and Civalek (2014a). However, it should be noted that the present theory uses only one variable whereas the theory of Akgöz and Civalek (2014a) uses three variables. It can be seen that the maximum deflections computed by the present theory and CT are higher than those given by EBT and MSGT while natural frequencies calculated by the present theory and CT are smaller than those given by EBT and MSGT and also these situations are more frequent for smaller shear modulus ratios and geometric ratios as $r = 10^{-6}$ and $L/D_0 = 50$. It can be observed that the results obtained by EBT and the present theory are almost equal for isotropic case and $L/D_0 = 500$. On the other hand, the differences between the results corresponding to EBT and the present theory are more obvious for the smaller geometric ratios ($L/D_0 = 50$), but they decrease for the larger ones, like $L/D_0 = 500$. In addition, it can be concluded that shear deformation effect becomes more important for small microtubules. Variations of maximum deflection and natural frequency ratios versus various geometric ratio and different shear modulus ratio are presented in Figs. 3 and 4, respectively. It is observed from these figures that the "*maximum deflection*" ratio is much larger than one while the natural frequency ratios are much smaller than one for smaller geometric ratios. However, these ratios tend to be closer to one with increasing aspect and shear modulus ratios, particularly for MSGT. It can also be emphasized that these ratios

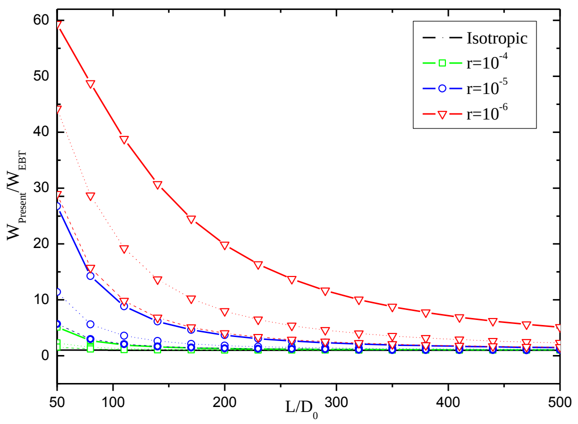

Fig. 3 Variation of maximum deflection ratio for various geometric ratio and different shear modulus ratio

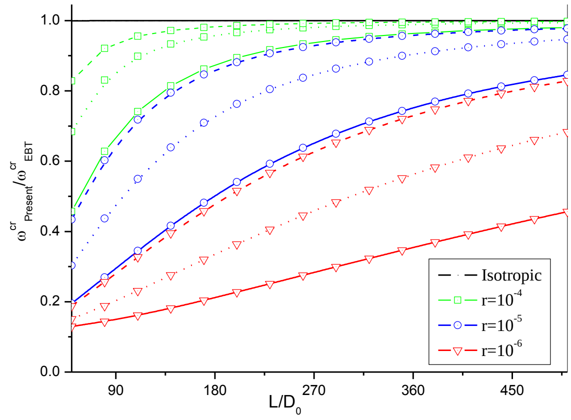

Fig. 4 Variation of natural frequency ratio for various geometric ratio and different shear modulus ratio

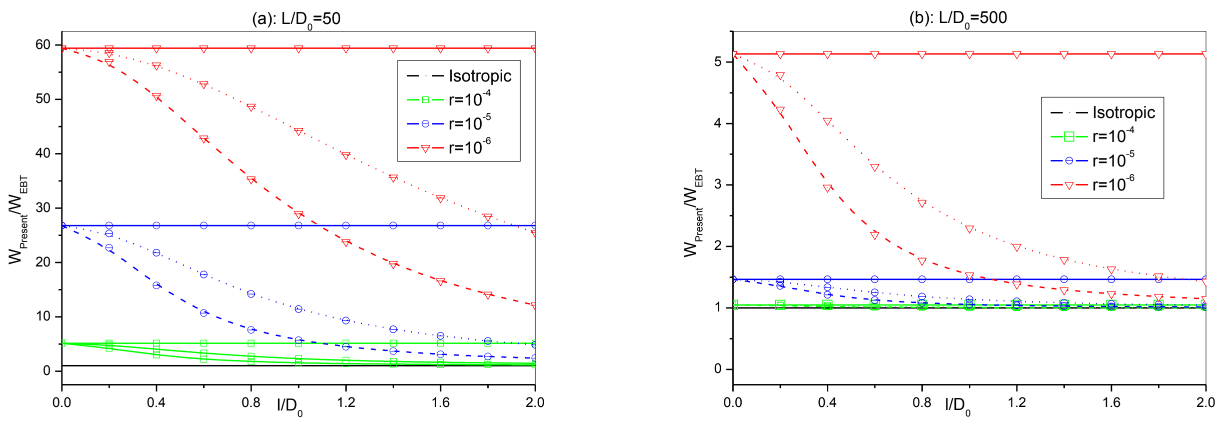

Fig. 5 Influences of length scale parameters on maximum deflection ratio for different shear modulus ratio (a) L/Do = 50, (b) L/Do = 500

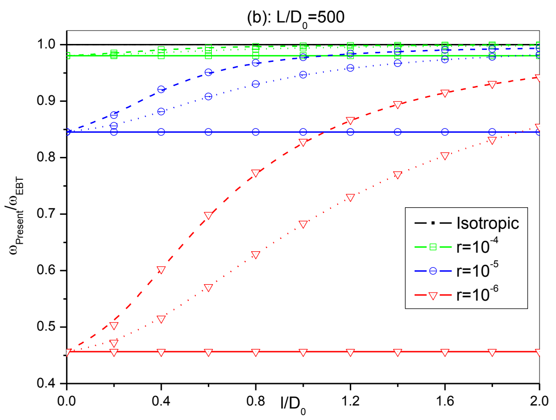

Fig. 6 Influences of length scale parameters on natural frequency ratio for different shear modulus ratio (a) L/Do = 50 (b) L/Do = 500

corresponding to isotropic case are almost equal to one. It can be deduced from the results that difference between elastic and shear modulus, resulting from composite structure and anisotropic molecular architecture of MTs, plays a considerable role on bending and dynamic properties of MTs.

Influences of material length scale coefficient-to-outer diameter ratio on maximum deflection and first natural frequency ratios of the simply supported MTs corresponding to various shear modulus ratios for $L/D_0 = 50$ and $L/D_0 = 500$ are illustrated in Figs. 5 and 6, respectively. It is seen that an increase in material length scale coefficient-to-outer diameter ratio leads to a decrement on influences of shear deformation while the shear deformation influences become more frequent by diminishing shear modulus ratio. In addition, it is clear that these ratios are closer to one for MSGT as a function of the increase in the material length scale parameter-to-outer diameter ratio. Also, it can be observed that the maximum deflection and natural frequency ratios for $L/D_0 = 50$ are always farther than those for $L/D_0 = 500$.

6. Conclusions

In this work, a microstructure-dependent "*shear deformation beam model*" is established for bending and free vibration investigation of microtubules on the basis of "*modified strain gradient elasticity theory*". The current single variable sinusoidal beam theory captures influences of shear deformation with no need for "*shear correction* *factors*” and this using only one variable as the Euler-Bernoulli beam theory. The equations of motion are determined by utilizing Hamilton’s principle. The bending and dynamic responses of simply supported isolated microtubules are investigated. Analytical solutions for deflections for point load at the midspan of the MTs and first three natural frequencies are obtained with the help of Navier solution technique. Influences of shear deformation, material length scale parameter, geometric ratio and shear modulus ratio on deflections and natural frequencies of microtubules are examined and discussed in detail. The results are compared with available results of open literature in conjunctions with CT and MCST. It is remarked that microstructure-dependent response is more important when material length scale parameters are close to the outer diameter of MTs. Classical beam models overestimate “*deflections*” while they underestimate “*natural frequencies*”. Similarly, single variable sinusoidal beam theory overestimates “*deflections*” while it underestimate “*natural frequencies*”, particularly for smaller geometric ratios. It can be observed that the beam models based on higher order elasticity models and simple beam model are stiffer than those based on classical theory and shear deformation beam models. In addition, it can be argued that the influences of shear deformation become larger because of the composite structure and anisotropic molecular architecture of MTs, particularly for smaller geometric ratios. An improvement of present formulation will be considered in the future work to consider other shear deformation models and other types of materials (Bouderba *et al*. 2013, Avcar 2015, 2016, 2019, Draiche *et al*. 2016, Bousahla *et al*. 2016, Daouadji 2017, Kar *et al*. 2017, Chikh *et al*. 2017, El-Haina *et al*. 2017, Lal *et al*. 2017, Bensattalah *et al*. 2018, Eltaher *et al*. 2018, Fakhar and Kolahchi 2018, Bourada *et al*. 2018, Ayat *et al*. 2018, Behera and Kumari 2018, Bakhadda *et al*. 2018, Faleh *et al*. 2018, Cherif *et al*. 2018, Panjehpour *et al*. 2018, Youcef *et al*. 2018, Rezaiee-Pajand *et al*. 2018, Kaci *et al*. 2018, Kadari *et al*. 2018, Selmi and Bisharat 2018, Narwariya *et al*. 2018, Bendaho *et al*. 2019, Boukhlif *et al*. 2019, Hellal *et al*. 2019, Draoui *et al*. 2019, Boutaleb *et al*. 2019, Zine *et al*. 2018, Adda Bedia *et al*. 2019, Bensattalah *et al*. 2019, Draiche *et al*. 2019, Hussain *et al*. 2019, Addou *et al*. 2019, Medani *et al*. 2019, Chaabane *et al*. 2019, Boulefrakh *et al*. 2019).

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