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Mechanical analysis of isolated microtubules based on a higher-order shear deformation beam theory

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ABSTRACT

In this paper, mechanical responses of isolated microtubules are investigated. Microtubules can be defined as bio-composite structures that are a component of the cytoskeleton in eukaryotic cells and play important roles in cellular processes. They have superior mechanical properties such as high rigidity and flexibility. In order to model the microtubules such as a hollow beam, a trigonometric shear deformation beam model is employed on the basis of modified strain gradient theory. The governing equations and related boundary conditions are derived by implementing Hamilton's principle. A detailed parametric study is performed to investigate the influences of shear deformation, material length scale parameter-to-outer radius ratio, aspect ratio and shear modulus ratio on mechanical responses of microtubules. It is observed that microstructure-dependent behavior is more considerable when material length scale parameters are closer to the outer diameter of microtubules. Also, it can be stated that effects of shear deformation become more significant for smaller shear modulus and aspect ratios.

1. Introduction

Microtubules (MTs) are one of the filamentary intracellular structures found in the cytoplasm together with actin and intermediate filaments. They are responsible in conducting of many basic functions in eukaryotic cells such as intracellular transport, ciliary and flagellar motility, cell division as well as mitosis and meiosis, providing the shape of cell during migration, separating chromosomes during cell division [1–3]. MTs are composed of two different type tubulins (α- tubulin and β- tubulin). Depending on the composite structure and anisotropic molecular architecture of them, MTs are about a hundred times stiffer than the other filaments and also they are quite flexible. MTs have a hollow cylindrical structure and typically occur from 13 parallel protofilaments *in vivo* whereas the number of protofilaments may vary in a range of 9 to 16 *in vitro* [4]. Protofilaments consist with self-assembling of tubulin heterodimers, comprising of α- and β-tubulins (see Fig. 1). The inner and outer diameters of MTs are about 15 nm and 25 nm, respectively and the length of MTs are in a range from ten nanometers to a hundred micrometers [5,6].

Because of the above-mentioned roles of MTs are related to mechanical properties of them, many experimental and theoretical studies have been performed by researchers. In experimental works [7–13], measurements have many difficulties and require very sensitive instruments. Therefore, theoretical models have been widely used to investigate the elastic properties and mechanical behaviors of MTs in recent times. It is experimentally observed that the bonds between adjacent protofilaments in the lateral direction are weaker than those in the longitudinal direction throughout protofilaments [14–16]. Moreover, the longitudinal elastic modulus of MTs is much larger than the shear and circumferential modulus [17–19]. A considerable difference between elastic and shear modulus may consist in quite anisotropic materials like wood and fiber-reinforced composites. These observations as well as composed of two tubulins show that MTs have nonhomogeneous structure and anisotropic properties. Consequently, effects of transverse shearing become more important on mechanical responses of MTs, especially for short MTs. In contrast to familiar concept of length-independent flexural rigidity of elastic structures (e.g. bar and beam), the flexural rigidity of MTs is length-dependent. It means that shear deformable continuum models like beam and shell are more convenient for modeling and analysis of MTs. Kis et al. [12] investigated anisotropic properties of single MTs and they found that the shear modulus is two orders of magnitude lower than elastic modulus. Kasas et al. [20] studied on mechanical properties of MTs with finite element method. Li et al. [21] and Wang et al. [22] introduced an orthotropic elastic shell model for MTs and they observed that length dependence of flexural rigidity is related to anisotropic elastic properties of MTs. Also, Ghavanloo et al. [23] and Daneshmand and Amabili [24] are developed a Bernoulli–Euler beam

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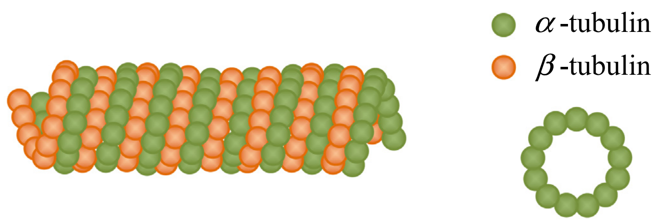

Fig. 1. Structure of a typical microtubule.

model and an orthotropic elastic shell model based on first-order shear deformation shell theory including the effects of the viscous cytosol and surrounding filaments to estimate the coupled oscillations of a single microtubule surrounded by cytoplasm, respectively. Shi et al. [25] and Tounsi et al. [26] proposed Timoshenko and parabolic shear deformation beam models respectively to take into account the influences of transverse shear deformation on mechanical properties of MTs. They compared with the results obtained by isotropic Bernoulli–Euler beam and orthotropic shell models and it is observed that the results predicted by shear deformable beam models are in good agreement with those evaluated by orthotropic shell model. Liew et al. [27] used a homogenization technique to compute the fictitious-bond energy in order to deal with the multi-atomic bio-composite structure. They predicted values for the fictitious-bond lengths between adjacent molecules in addition to lateral and longitudinal elastic modulus of MTs. Also, atomistic continuum models for mechanical analysis of MTs have been presented [28–31].

However, some experimental studies have been demonstrated that the existing size effect plays an important role on mechanical behaviors of small-sized structures [32–34]. The conventional (classical) continuum theories have no intrinsic or material length scale parameters and fail to estimate the size dependent behaviors of micro- and nano-scaled structures. Hence, various non-classical (higher-order) continuum theories have been proposed to predict the mechanical behaviors of small-sized structures such as couple stress theory [35–37], micropolar theory [38], nonlocal elasticity theory [39,40] and strain gradient theories [41–43].

The modified strain gradient theory [33] is one of the above-mentioned higher-order continuum theories in which strain energy density contains second-order deformation gradients (dilatation gradient vector, deviatoric stretch and symmetric rotation gradient tensors) in addition to first-order deformation gradient (symmetric strain tensor). For linear elastic isotropic materials, the formulations and governing equations include three additional material length scale parameters related to higher-order deformation gradients besides two classical ones. This popular theory has been employed to investigate mechanical behaviors of size-dependent one-dimensional structures like microbars [44–49] and microbeams [50–64].

As stated before, the length and diameter of MTs are in the order of micrometers and nanometers, respectively. In this regard, modeling and analysis of MTs based on non-classical (higher-order) continuum theories have been become more popular in recent times. Gao and Lei [65] and Fu and Zhang [66] investigated the persistence length and buckling responses of MTs based on nonlocal elasticity theory and modified couple stress theory, respectively. Heireche et al. [67] introduced a nonlocal Timoshenko beam model for free vibration of protein MTs in viscoelastic surrounding cytoplasm. The buckling behaviors of microtubules in living cells have been studied by Gao and An [68] based on nonlocal anisotropic shell theory. Shen [69–71] developed nonlocal shear deformable shell models for linear and nonlinear analysis of MTs. Furthermore, static and dynamic analysis of MTs investigated based on Bernoulli–Euler beam and such non-classical continuum theories [72–75].

In this paper, mechanical responses of microtubules, one of the main components of the cytoskeleton in living cells, are investigated. In order to model the microtubules such as a hollow cylindrical beam, a trigonometric shear deformation beam model is developed on the basis of modified strain gradient elasticity theory. The governing differential equations and corresponding boundary conditions are obtained with the aid of Hamilton's principle. The static bending, buckling and free vibration responses of simply supported microtubules are investigated. A detailed parametric study is performed to investigate the influences of shear deformation, material length scale parameter-to-outer radius ratio, aspect ratio on mechanical responses of MTs. Additionally, effects of shear modulus ratio corresponding to the large difference between elastic and shear modulus due to difference in bond strengths between longitudinally (along the protofilaments) and laterally (between adjacent protofilaments) bonds arising from composite structure and anisotropic molecular architecture of MTs are also investigated. Moreover, the results are compared with those evaluated by simple beam theory in conjunctions with classical and modified couple stress theories.

2. The modified strain gradient elasticity theory

The modified strain gradient elasticity theory (MSGT) has been proposed by Lam et al. [33] is one of the popular higher-order (non-classical) continuum theories. Unlike conventional (classical) continuum theories, this theory takes into consideration some higher-order strain gradient in addition to classical strain tensor in formulations as dilatation gradient vector, deviatoric stretch gradient and symmetric rotation gradient tensors. The strain energy U for the modified strain gradient theory can be written with infinitesimal deformations as [33]

$$U = \frac{1}{2}\int_0^L \int_A \left(\sigma_{ij}\varepsilon_{ij} + p_i\gamma_i + \tau^{(1)}_{ijk}\eta^{(1)}_{ijk} + m^s_{ij}\chi^s_{ij}\right) dA dx \tag{1}$$

where ε_{ij}, γ_i, $\eta^{(1)}_{ijk}$ and χ^s_{ij} indicate the components of the strain tensor $\boldsymbol{\varepsilon}$, the dilatation gradient vector γ, the deviatoric stretch gradient tensor $\boldsymbol{\eta}^{(1)}$ and the symmetric rotation gradient tensor $\boldsymbol{\chi}^s$, respectively and are described as following

$$\varepsilon_{ij} = \frac{1}{2}\left(u_{i,j} + u_{j,i}\right) \tag{2}$$

$$\gamma_i = \varepsilon_{mm,i} \tag{3}$$

$$\eta^{(1)}_{ijk} = \frac{1}{3}\left(\varepsilon_{jk,i} + \varepsilon_{ki,j} + \varepsilon_{ij,k}\right) - \frac{1}{15}\left[\delta_{ij}\left(\varepsilon_{mm,k} + 2\varepsilon_{mk,m}\right) + \delta_{jk}\left(\varepsilon_{mm,i} + 2\varepsilon_{mi,m}\right) + \delta_{ki}\left(\varepsilon_{mm,j} + 2\varepsilon_{mj,m}\right)\right] \tag{4}$$

$$\chi^s_{ij} = \frac{1}{2}\left(\theta_{i,j} + \theta_{j,i}\right) \tag{5}$$

$$\theta_i = \frac{1}{2}e_{ijk}u_{k,j} \tag{6}$$

in which u_i denotes the components of displacement vector $\mathbf{u}$ and θ_i denotes the components of rotation vector $\boldsymbol{\theta}$, also δ and e_{ijk} are the Kronecker delta and permutation symbols, respectively. Furthermore, the components of Cauchy stress tensor $\boldsymbol{\sigma}$ and higher-order stress tensors $\mathbf{p}$, $\tau^{(1)}$ and $\mathbf{m}^s$ (conjugated with $\boldsymbol{\varepsilon}$, γ, $\boldsymbol{\eta}^{(1)}$ and $\boldsymbol{\chi}^s$ respectively) are expressed as following [33]

$$\sigma_{ij} = \lambda\delta_{ij}\varepsilon_{mm} + 2G\varepsilon_{ij} \tag{7}$$

$$p_i = 2Gl_0^2\gamma_i \tag{8}$$

$$\tau^{(1)}_{ijk} = 2Gl_1^2\eta^{(1)}_{ijk} \tag{9}$$

$$m^s_{ij} = 2Gl_2^2\chi^s_{ij} \tag{10}$$