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Application of strain gradient elasticity theory for buckling analysis of protein microtubules

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ABSTRACT

In this paper, size effect of microtubules (MTs) is studied via modified strain gradient elasticity theory for buckling. MTs are modeled by Bernoulli–Euler beam theory. By using the variational principle, the governing equations for buckling and related boundary conditions are obtained in conjunctions with the strain gradient elasticity. The size effect for buckling analysis of MTs is investigated and results are presented in graph form. The results obtained by strain gradient elasticity theory are discussed through the numerical simulations. The results based on the modified couple stress theory, nonlocal elasticity theory and classical elasticity theories have been also presented for comparison purposes.

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1. Introduction

Micro and nanobeams have been widely used in nano and microsized systems and devices such as biosensors, nanowires, atomic force microscope, microactuators, nano probes, micro electromechanical, ultra thin films and nano electromechanical systems [1].

Another important micro structure is the protein microtubules in living cell. It is well known that microtubules (MTs), microfilaments and intermediate filaments are the main components of cytoskeleton. MTs are protein organized in a network that is interconnected with microfilaments and intermediate filaments to form the cytoskeleton structures [2]. The mechanical properties of MTs play an important role in process such as cell division and intracellular transport [3,4]. MTs are the most rigid of the cytoskeletal filaments and have the most complex structure. The structure of MTs is cylindrical and it typically involves 13 parallel protofilaments which are connected laterally into hollow tubes. MTs are considered as hollow cylinders having 25 nm external and 15 nm internal diameters. The length of MTs can vary from tens of nanometers to hundreds of microns. Furthermore, MTs are considered as self-assembling biological nanotubes that are essential for cell motility, building the cytoskeleton, cell division

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and intracellular transport. The average Young's modulus of MTs is \sim 2.0 GPa [5–10]. Among the three types of cytoskeletal filaments, MTs are the most rigid. It is also stated that the bending rigidity of MTs is about 100 times that of intermediate and actin filaments. It is observed that the size effect has a major role on static, buckling and dynamic behavior of micro- and nano-scaled structures and can't be negligible. This size effect has not been interpreted by classical (Cauchy) elasticity. After that, higher order elasticity theories have widely been used by researchers. There have been a number of experimental and mathematical studies in recent past ten years dealing with the mechanical properties of MTs [11–17]. Wang et al. [18] investigate the buckling analysis of MTs via orthotropic elastic shell. Buckling analysis of MTs is presented by Gao and An [19] based on the anisotropic shell model. Ece and Aydogdu [20] used nonlocal elasticity for in-plane vibration analysis of double-walled carbon nanotubes. Small scale effects on the mechanical behaviors of protein MTs based on the nonlocal elasticity theory is investigated by Gao and Lei [21]. Buckling and postbuckling analyses of MTs have been detailed investigated by Shen [22-25] based on the nonlocal shell model. Recently, a modified type of couple stress theory was proposed by Yang et al. [26]. There is only one additional material length scale parameter in this theory and also couple stress tensor is symmetric. This modified couple stress theory is more useful than classical one due to these features. The modified strain gradient elasticity theory is another higher-order continuum theory, which was proposed by Lam et al. [27] contains





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a new additional equilibrium equation besides the classical equilibrium equations and also five elastic constants (two classical and three non-classical) for isotropic linear elastic materials. Both the strain gradient elasticity and couple stress theories are included the second-order displacement gradients. Then, a new Bernoulli-Euler beam model was developed by Park and Gao [28] by using the modified couple stress theory for bending. After this, modified couple stress and strain gradient elasticity theories have been widely applied to static and dynamic analysis of beams and plates [29–37]. Equilibrium and static deflection for bending of nonlocal nanobeams are investigated in detail by Lim and Wang [38]. In some of the recent published works, for example [39-47], the importance of using nonlocal theory has been addressed and very detailed results were presented. More recently, buckling analysis of nano-sized structures has been reviewed by Wang et al. [48] in detail. Buckling instability of nanobeams is investigated in conjunction with the stiffness strengthening effects of using the nonlocal elasticity theory is investigated [49]. Cylindrical shell model is also adopted for modeling of nanostructures [50,51]. By using the higher-order continuum approach, analyses of microsized mechanical and biological systems are also investigated by present authors [52-56].

In the present work, the consistent governing equations for the buckling for MTS are derived using strain gradient elasticity and variational approach via Bernoulli–Euler beam theory. To the best knowledge of authors, it is the first time the strain gradient elasticity and couple stress theories have been successfully applied to MTs for buckling analysis. The influences of the length scale parameter, on the buckling characteristics of MTs have been discussed in detailed.

2. Strain gradient formulation for stability

The strain energy U in a linear elastic isotropic material occupying region Ω based on the modified strain gradient elasticity theory can be written by [27]:

$$U = \frac{1}{2} \int_{\Omega} \left(\sigma_{ij} \varepsilon_{ij} + p_i \gamma_i + \tau^{(1)}_{ijk} + m^s_{ij} \chi^s_{ij} \right) \mathrm{d}\nu, \tag{1}$$

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

$$\varepsilon_{mm,i} = \gamma_i,$$
(3)

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

$$\chi_{ij}^{s} = \frac{1}{2} (e_{ipq} \varepsilon_{qj,p} + e_{jpq} \varepsilon_{qi,p}).$$
(5)

where u_i is the displacement vector, ε_{ij} is the strain tensor, $\varepsilon_{mm,i}$ is the dilatation gradient vector, $\eta_{ijk}^{(1)}$ is the deviatoric stretch gradient tensor, χ_{ij}^{s} is the symmetric rotation gradient tensor, δ_{ij} is the Kronecker delta and e_{ijk} is the permutation symbol. The stress measures: σ_{ij} is the classical stress tensor and p_i , $\tau_{ijk}^{(1)}$, m_{ij}^{s} are the higher order stresses, also ε'_{ij} is deviatoric strain, respectively, defined as [27]:

$$\sigma_{ij} = k \delta_{ij} \varepsilon_{mm} + 2\mu \varepsilon'_{ij}, \tag{6}$$

$$p_i = 2\mu l_0^2 \gamma_i, \tag{7}$$

$$\tau_{ijk}^{(1)} = 2\mu l_1^2 \eta_{ijk}^{(1)},\tag{8}$$

$$m_{ij}^s = 2\mu l_2^2 \chi_{ij}^s, \tag{9}$$

$$\varepsilon_{ij}' = \varepsilon_{ij} - \frac{1}{3} \varepsilon_{mm} \delta_{ij}. \tag{10}$$

where *k* is bulk module, μ is shear module and l_0 , l_1 , l_2 are additional material length scale parameters related to dilatation gradients, deviatoric stretch gradients and rotation gradients, respectively. By using the above equations, the strain energy *U* in equation (1) can be rewritten as:

$$U = \frac{1}{2} \int_{0}^{L} \left[B \cdot (w'')^{2} + D \cdot (w''')^{2} \right] dx, \qquad (11)$$

where,

$$B = EI + 2\mu A l_0^2 + \frac{8}{15} \mu A l_1^2 + \mu A l_2^2, \quad D = I \left(2\mu l_0^2 + \frac{4}{5} \mu l_1^2 \right),$$
(12)

I and *A* are the moment of inertia and cross section area of the beam, respectively. Detailed derivation for strain energy statement in equation (11) is presented by present authors [56]. When we consider in addition the effect of the axial compressive force *N*, one obtains the following expression for the strain energy in equation (11):

$$U = \frac{1}{2} \int_{0}^{L} \left[B \cdot (w'')^{2} + D \cdot (w''')^{2} \right] dx - \frac{1}{2} \int_{0}^{L} N(w')^{2} dx.$$
(13)

Finally, the governing equation of MTs for buckling as well as all possible boundary conditions can be determined using the following variational principle:

$$\delta(U - W) = \int_{0}^{r} \left[B \cdot w^{(4)} - D \cdot w^{(6)} + Nw'' \right] \delta w dx + \left[- B \cdot w''' + D \cdot w^{(5)} - Nw' - V \right] \delta w \Big|_{0}^{L} + \left[B \cdot w'' - D \cdot w^{(4)} - M_{c} \right] \delta w' \Big|_{0}^{L} + \left[D \cdot w''' - M_{nc} \right] \delta w'' \Big|_{0}^{L} = 0.$$
(14)

It can be seen clearly from the above variational equation that each term must be equal to zero. Hence, the governing equation for buckling is given by Akgöz [52]:

$$B \cdot w^{(4)} - D \cdot w^{(6)} + N w'' = 0, \tag{15}$$

and the boundary conditions at x = 0,L;

$$V = D \cdot w^{(5)} - B \cdot w^{\prime\prime\prime} - Nw' \text{ or } \delta w = 0$$

$$M_{c} = B \cdot w^{\prime\prime} - D \cdot w^{(4)} \text{ or } \delta w' = 0$$

$$M_{nc} = D \cdot w^{\prime\prime\prime} \text{ or } \delta w^{\prime\prime} = 0.$$
(16)

Similarly, when the additional material length scale parameters l_0 and l_1 in the modified strain gradient elasticity theory equal to

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