Applied Mathematics and Computation 321 (2018) 313–332

Contents lists available at ScienceDirect

Applied Mathematics and Computation

journal homepage: www.elsevier.com/locate/amc

Computational vibration and buckling analysis of microtubule bundles based on nonlocal strain gradient theory

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ARTICLE INFO

Keywords:
Microtubule bundles
Nonlocal strain gradient theory
Finite element method
Surface effects
Pasternak foundation

ABSTRACT

A nonlocal strain gradient model is proposed to study buckling and vibrational responses of microtubules in axons with attention to different size effect parameters based on finite element method. Supporting effects of surrounding cytoplasm and MAP Tau proteins are considered. Microtubules are modeled as elastically connected improved Timoshenko nano-beams resting on a two-parameter Pasternak foundation. Differential equations are discretized using Galerkin method. Finally, two eigenvalue problems are solved to achieve critical buckling loads and frequencies of single and doubled-microtubule systems. The nonlocal strain gradient model is employed in order to show both hardening and softening effects of structural stiffness, based on relative magnitudes of nanoscale parameters. Influence of size effects, including nonlocal nanoscale parameter, gradient coefficient and surface effects, are examined for various boundary conditions and some benchmark results are reported. It is observed that these effects are more prominent at higher modes. Based on presented numerical results, MAP Tau proteins strengthen doubled microtubule systems to bear 11.7% more buckling load than a single microtubule. Furthermore, vibration frequencies of microtubules depend on their physical surrounding condition in cell; such as cell matrix and membrane, and since microtubules could be employed as biosensors, this property may be used in order to detect malignant tumors, based on vibrational damping.

1. Introduction

Traumatic brain injury (TBI) is one of the main death causes in incidents worldwide. In some cases, these axonal damages are microscopic and todays imaging techniques are incapable of detecting these rapid deformations in neurons. In these kinds of damages, computational mechanics can effectively model brain tissue behavior and recognize the damage mechanism. As largest cells in body, mechanical integrity of neurons depend mainly on microtubules for cell division, growth and migration [33,36,42]. Microtubules have the greatest flexural rigidity among filamentous network proteins. It has been reported that they can bear 100 times greater compressive loadings than actin filaments and intermediate filaments (Waterman & Salmon, [27,38,49,50]). Microtubules are all made up of 13 longitudinal repeating units, they have cylindrical shapes and their inner and outer diameters are about 15.4 nm and 25 nm with a length up to 20 μm [42]. Buckling of microtubules has been examined in some computational and experimental studies in variety of living cells and the role of supporting cytoskeletal is investigated. It has been presented that MTs have a first mode large-wave length buckling in vitro, while they

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https://doi.org/10.1016/j.amc.2017.10.050
0096-3003/

buckle in shorter wave lengths when supporting filamentous network couples with them as in vivo observations ([37]; Mizushima et al. [5,10,14,15,18,22,23,25,31,32,34,35,39,43,49]). Kurachi et al. [37] employed optical trapping technique in order to do direct loading on a single microtubule and concluded that buckling load depends severely on microtubule's length. Brangwynne et al. [5] studied influence of supporting cytoplasm on buckling wave length and critical load and reported interesting results.

Bead-spring models also were used in a number of cases for examining mechanical characteristics of axonal MTs in various loading conditions. Peter & Mofrad [47] studied tensile of axonal MTs in viscos cytoplasm. Soheilypour et al. [38] investigated buckling of MT bundles and reported their short-wave length and decaying behavior. Torsion of axonal MTs also was researched theoretically by Lazarus et al. [38]. In all these studies, MAP Tau proteins modeled as linear springs and their distance with each other on microtubules was studied. Molecular dynamics and atomistic simulations are also used by researchers for modeling nano scale systems, but they are difficult to perform and have too much computational costs [10].

Considering size effects of microtubules, several size-dependent theories such as Cosserat elasticity, couple stress theory, strain gradient elasticity, surface energy theory, and stress gradient theories are proposed and used. In the past decade, Eringen's nonlocal theory [19] has been used a lot by researchers [1,7,8,10–12,17,26,30,40]. Based on this theory, stress at one point of a continuum is a function of strain of that specific point and all strains of other points of that continuum, which distinguishes nonlocal continuum theory from classical theory. By using nonlocal theory, one can easily incorporate long range cohesive forces between atoms and molecules in continuum model. Civalek and Demir [10] modeled a single MT on elastic foundation and examined static instability for various types of MTs in different buckling modes. Demir [11] investigated free vibration of carbon nanotubes (CNTs) by shear deformable beam theory and discrete singular convolution technique. Pradhan and Mandal [45] employed a finite element method studying buckling, vibration and bending of carbon nanotubes using nonlocal elasticity theory and applying thermal environment. In some cases, Eringen's theory has been used on vibrational examination of single-walled and double-walled carbon nanotubes [3,4,17]. Further using nonlocal elasticity and nonlocal discrete theory, Demir and Civalek [12] proposed a finite element model for studying of Torsional and axial frequencies of MTs. Thermal vibrations of nano beams on Pasternak foundation also was investigated by Demir and Civalek [13] using finite element method and frequencies for variety of modes were reported. Akgöz and Civalek [8] presented a strain gradient model using Euler-Bernoulli beam theory for buckling of functionally graded material (FGM) micro beams and studied various boundary conditions. In another paper, Akgöz and Civalek [9] proposed a modified strain gradient theory to investigate size effects and different beam theories in buckling of a beam embedded in two-parameter elastic foundation. They studied length to diameter and shear correction factor effects through parabolic beam theory (PBT), sinusoidal beam theory (SBT) and Timoshenko beam theory (TBT).

Based on surface elasticity theory, the surface energy of an elastic medium depends on some deeper layers of atoms. Although this effect might be negligible in regular sized structure, its existence in nano/micro structures carries lots of weights [29]. Farajpour et al. [21] provided an analytical approach to examine buckling of bundles of MTs considering surface effects. Nonlocal strain gradient theory has been employed recently by researchers in order to study influence of nonlocality and strain gradient parameter, simultaneously, on the nano/micro structures. Barati [2] used this theory to investigate thermal loading on nonporous nano-beams. Ebrahimi et al. [16] employed a shear deformation plate theory to examine wave propagation in functionally graded materials. Zhu and Li [52] proposed a size-dependent integral elasticity model to study tension in a small scaled rod. Xu et al. [51] presented a nonlocal strain gradient model to achieve vibrational response of Euler-Bernoulli beam, using weighted residual method. Nonlinear vibration of functionally graded materials, considering sized effects was investigated by Simsek [48] and a closed-from solution was achieved. Free vibration of nano-beams, using size-dependent sinusoidal shear deformation beam model, has been developed by Lu et al. [28].

With all these great scientific jobs mentioned earlier, to the best of authors knowledge, there remains an empty space for finite element examination of free vibration and buckling of MT bundles using nonlocal strain gradient theory considering surface energy effects in the literature. In this paper, a MATLAB code has been developed based on finite element method and using improved Timoshenko beam elements for examining vibration and buckling of axonal MTs. Despite random positioning of MTs in other cells, axonal MTs are well patterned structures, which are connected to each other by MAP Tau proteins. These proteins provide coupling effects including transverse displacements and shearing force. Microtubules are also benefited from lateral support of actin filaments and intermediate filaments. MAP Tau proteins and filamentous network of cytoplasm play great role in axons stability. So in this study, they are considered by Pasternak model. This research is validated by some experimental and computational results reported in the literature and excellent agreements are reached. Finally, parametric results for vibrational frequencies and critical buckling loads in various modes and boundary conditions have been obtained, which will be useful for future studies.

2. Nonlocal strain gradient elasticity

Fig. 1a shows schematic of a neuron and its axon and other corresponding components. A zoomed-in view of the axon illustrates microtubule bundles connected to each other via MAP Tau proteins (Fig. 1b). In this study, in order to apply the effects of MAP Tau proteins and cytoplasm matrix, microtubules are modeled as Timoshenko beams on Pasternak foundation (Fig. 2a) that are connected to each other by spring elements modeled using Pasternak layers (Fig. 2b).

Based on the Eringen's nonlocal elasticity theory, stress at a special point is a function of strain at that specific point and also the whole elastic body. This theory is capable of predicting stiffness softening of structure with respect to nonlocal size