Advances in Nano Research, *Vol. 17, No.5 (2024) 401-408*
https://doi.org/10.12989/anr.2024.17.5.401

Nonlocal orthotropic shell model for buckling of microtubules embedded within elastic medium

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(*Received August 11, 2021, Revised August 30, 2024, Accepted September 10, 2024*)

Abstract. Nonlocal influences are taken into account when studying the buckling behavior of protein microtubules in the elastic medium. The protein microtubules are modeled using the Winkler model as an orthotropic shell. Combining the two models, a new nonlocal orthotropic Winkler model is created that accounts for nonlocal influences in order to study the buckling of protein microtubules within the elastic medium. The wave propagation approach, a well-known numerical technique, is used to solve the governing equations. The primary goal of the current work is to examine microtubule buckling against dimensionless axial wavelength. This findings and observations supported the conclusions of the earlier investigations.

Keywords: buckling; elastic medium; microtubule; nonlocal orthotropic Winkler-like model; wave propagation approach

1. Introduction

Actin filaments (MFs), microtubules (MTs), and intermediate filaments (IFs) are the major building blocks of cytoskeletal structures. Among these, MTs are crucial for a wide range of cellular processes in both prokaryotes and eukaryotes, including mitosis (Albert, 1994, Zhang *et al.* 2023). Chromosomes, proteins, and other organelles are separated by it (Wang *et al.* 2024, Wu *et al.* 2024). Additionally, they make long-distance intracellular transport possible (Vale, 2003). They provide the force needed to support motor proteins, which are necessary for shape changes and cell movement. In addition to giving cells their mechanical strength, MTs play a critical role in the delivery of anticancer medications and other failing structures (Jordan and Wilson, 2004, Su *et al.* 2024, Zhang *et al.* 2024a).

They contribute significantly to exceptional small-scale resilience and exhibit sufficient resistance to bending on a large-scale basis (Jiang *et al.* 2016). The stiffest elements of the cytoskeletal framework are thought to be MTs. In addition to their importance in biological functions, MTs mechanical properties are also crucial for the design of molecular shuttles and force studies in small ranges up to Pico-Newton for the persistent shrinking of lab-on-a-chip instruments (Hess *et al.* 2002, Nitta and Hess 2005). Tubulin protein heterodimers with a long, hollow, cylindrical shape make up of MTs. The longitudinal bounds between tubulin protein heterodimers along the proto-filaments (PFs) are more stronger than the lateral bindings between adjacent PFs, according to certain investigations (Needleman *et al.* 2004, Nogales *et al.* 1998). According to Wang *et al.* (2006), the longitudinal elastic modulus of MTs is noticeably greater than the shear modulus and the circumferential elastic modulus.

Numerous studies, both in vitro and in vivo, have been conducted to examine the mechanical behaviors of MTs, particularly the buckling behavior (Kurachi *et al.* 1995), Elbaum *et al.* 1996, Needleman *et al.* 2004, Brendan *et al.* 2006) and composite construction. In vivo research has addressed the MT bending at shorter wavelengths caused by axial compression (Brangwynne *et al.* 2006). According to Elbaum *et al.* (1996), compressive force of the MTs in vivo is of the 5th order of magnitude of 100 pN, although in vitro investigations show extended wave length buckling of a single microtubule and significantly smaller compression. The cytoplasmic short wavelength of MTs buckles with large compression forces. In order to reveal the buckling behaviors in the natural surrounding medium, Li (2008) effectively described the buckling behaviors of short wavelength microtubules and modeled the MTs embedded in viscous medium using the Euler beam model. To address the mechanical characteristics of MTs embedded in a three-dimensional isotropic linear elastic medium, another model resembling a cylindrical tube has been developed (Jiang and Zhang 2008). The traditional elastic shell model was

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http://www.techno-press.org/?journal=journal=anr&subpage=5
ISSN: 2287-237X (Print), 2287-2388 (Online)

designed to describe the local mechanical behavior and to characterize three-dimensional structures. In order to investigate the radical pressure and buckling modes of MTs under uniform external axial compressive stresses, this model was extensively used in MT modeling (Gao *et al.* 2010). This approach has been further developed to analyze the torsion and bending in MTs (Yi *et al.* 2008). To experience transverse sharing and investigate the impact of transverse sharing on shell-like mechanics of MTs, an orthotropic elastic shell model has been suggested (Gu *et al.* 2009). A suitable adaptation of the traditional cracked-beam theory is used to simulate the cracked beam. It consists of two sub-beams joined by a massless elastic rotational spring. An optimization technique and a physical-constrained decomposition method for various architectures (Wang *et al.* 2024, Yang *et al.* 2024). The persistent length of microtubules is examined by the author using an anisotropic elastic shell theory (Gao *et al.* 2010). In terms of MTs elastic constants, he put up a close form solution that may be useful in understanding a number of pertinent experimental occurrences. Concurrently, research has been done on the dynamic behaviors of MTs and how cytoplasm affects them. In order to investigate the elastic vibrations of MTs in fluids, the shell fluid-model was also put out (Sirenko *et al.* 1996). The MTs surface ionic charge layer can lessen the viscosity effect of the cytosol, allowing the cytosol and MTs to slip past each other, as demonstrated by Ponkory's studies (Pokorný 2003, 2004). An orthotropic elastic shell model was presented by Wang *et al.* (2009) in order to examine the dynamic behavior of MTs implanted in cytosol. It has been investigated that the size of a material affects its qualities in a nanoscale structure (Ece and Aydogdu 2007, Wang and Liew 2007, Reddy and Pang 2008, Murmu and Pradhan 2009). MTs mechanical behavior has been studied using conventional continuum models. The tiny scale action of MTs cannot be adequately described by the standard models. The non-local elastic theory (Eringen 1983) postulates that the state of strain at each continuum point should determine the condition of stress at that point. This theory was not the same as the conventional, classical theory of elasticity. This theory allows for the consideration of both small-scale effects and long-range forces between atoms. Only a tiny number of MT studies consider the small scale impacts. Nonlocal Timoshenko beam model was recently presented by the author in reference (Gao and Lei 2009) to determine the buckling behaviors of MTs and persistence length. For the first time, the small scale influences on MTs mechanical behaviors are examined in this model. Nonlocal shear shall model was established by (Shen 2010b) to investigate the post buckling and static buckling behaviors of MTs in an elastic medium. Because of this model, the small scale parameter's value of nonlocal parameter, was estimated and contrasted with the findings of the experiments.

The post buckling behaviors and radial buckling of MTs subjected to radial load have been explored in the nonlocal shear shell model (Shen 2010b). Studies have been conducted on the bending behaviors of MTs under the nonlocal Euler Bernoulli beam model, taking into account small-scale effects and MT free vibration (Civalek *et al.* 2010). Many material scientists (Wang *et al.* 2007, Gupta *et al.* 2010, Swain *et al.* 2013, Xu *et al.* 2023) have recently conducted studies on the vibration of SWCNTs. A number of researchers have investigated frequency analysis using various techniques (Bilouei *et al.* 2016, Golabchi *et al.* 2018, Zamani *et al.* 2017, Zhang *et al.* 2023, 2024b). There is a prediction for multi-state fusion with reduced structural interface (Wang *et al.* 2024, Zhang *et al.* 2023).

MFs exhibit flexibility and relative strength, withstanding filament fracture due to Nano newton tensile forces and buckling caused by multi-Pico newton compressive forces (Barany 2001, Elzinga 1973, Collins *et al.* 1973). According to Otterbein *et al.* (2001), Graceffa *et al.* (2001), Holmes *et al.* (1990), Pop *et al.* (1990), myosin II molecular motors are likely responsible for one end of the MFs elongation and contraction during the induction of cell motility. Furthermore, the thin filaments function as tensile platforms for the ATP-dependent pulling action of myosin in the muscle contraction and pseudopod advancement, as part of actinmyosin-driven contractile molecular motors (Gunning *et al.* 2015, Ghoshdastider *et al.* 2015, Oriol *et al.* 1977, Dubord *et al.* 1977). MFs have a robust, adaptable structure that facilitates cell mobility (Bennett and Baines 2001). The majority of MFs are found beneath the plasma membrane, where they organize into a network that supports cells mechanically, shapes the cell, and permits surface movement. This network enables cells to migrate, take up particles, divide, and distribute stress in composite pipes (Yao *et al.* 2024, Ghoshdastider *et al.* 2015, Jiang *et al.* 2015). They move along other proteins termed myosin fibers in skeletal muscle to cause a cell to contract. The use of various approaches for nonlinear modeling has been observed in recent times by some researchers (Tohidi *et al.* 2018, Arefi and Zenkour, 2017, Arani *et al.* 2018, Krommer *et al.* 2016, Yeh 2016) as well as for other structures (Boussoula *et al.* 2020, AlSaleh and Fuggini 2020, Lee *et al.* 2019, Zahrai and Kakouei 2019, Poplawski *et al.* 2019, Akbaş 2018a, b, Sedighi and Daneshmand 2014, Asghar *et al.* 2020, Hussain and Naeem 2019, Fatahi-Vajari *et al.* 2019, Khadimallah *et al.* 2020a, b, Banoqitah *et al.* 2022, Hussain 2022, Qazaq *et al.* 2022, Muzamal 2022, Arshad *et al.* 2024, Hussain *et al.* 2020a, b, 2024, Huang *et al.* 2022, Zhao *et al.* 2022).

Many researchers and scientist did notable work on the buckling behavior of MTs but somehow ignored the actual environment of MTs using classical theory of elasticity. MTs are naturally embedded in an elastic medium, so this medium should be taken into account for the accurate modeling and physically significant results. A free body can buckle more rapidly and easily as compared to the body embedded in any denser medium. Scientifically, an elastic medium around a body reduces the magnitude of buckling. Also the nonlocal effects cannot be ignored for such problems of mechanics. Therefore, the modeling of embedded MTs for physically accurate and reliable results using nonlocal theory is explored.

2. Formulations and models

The nonlocal orthotropic elastic shell model will be utilized to examine the buckling behavior of metal thin films. The Winkler model will be used to model the surrounding medium of MTs. By merging these models, we will create a nonlocal orthotropic Winkler model. To determine the dispersion relations for embedded MTs, we shall employ the wave propagation technique.

2.1 Nonlocal orthotropic Winkler model

According to Wang *et al*. (2006), a non-local Winkler-like model is used to investigate the buckling of MTs under natural conditions.

$$\begin{aligned}&\frac{\partial^2\gamma_1}{\partial{\lambda_2}^2}-\frac{1}{(\eta^2+1)\chi_2}\left[-1+\hat{N}\frac{(1-e_0a)^2\nabla^2}{\Omega}\right]\frac{\partial^2\gamma_1}{\partial{\lambda_1}^2}\\&+\frac{(\zeta_1+\chi_2)}{(\eta^2+1)\chi_2}\frac{\partial^2\gamma_2}{\partial\lambda_1\partial\lambda_2}+\\&\frac{1}{(\eta^2+1)\chi_2}\left[\zeta_1\frac{\partial}{\partial\lambda_1}+\eta^2\left(\chi_2\frac{\partial^3}{\partial\lambda_1\partial{\lambda_2}^2}-\frac{\partial^3}{\partial{\lambda_2}^3}\right)\right]\gamma_3=0\end{aligned}\tag{1}$$

$$\begin{aligned}&\left[\frac{\partial^2}{\partial\lambda_1\partial\lambda_2}\right]\gamma_1\\&+\frac{1}{(\zeta_1+\chi_2)}\left[\begin{matrix}\chi_2(1+3\eta^2)\dfrac{\partial^2}{\partial{\lambda_1}^2}\\-\dfrac{\hat{N}}{\Omega}((1-e_0a)^2\nabla^2)\dfrac{\partial^2}{\partial{\lambda_1}^2}+\chi_1\dfrac{\partial^2}{\partial{\lambda_2}^2}\end{matrix}\right]\gamma_2\\&+\frac{1}{(\zeta_1+\chi_2)}\left[\chi_1\frac{\partial}{\partial\lambda_2}-\eta^2(\zeta_1+3\chi_2)\frac{\partial^3}{\partial{\lambda_1}^2\partial\lambda_2}\right]\gamma_3=0\end{aligned}\tag{2}$$

$$\begin{aligned}&\left[\zeta_1\frac{\partial}{\partial\lambda_1}-\eta^2\left(\frac{\partial^3}{\partial{\lambda_1}^3}-\chi_2\frac{\partial^3}{\partial\lambda_1\partial{\lambda_2}^2}\right)\right]\gamma_1\\&+\left[\chi_1\frac{\partial}{\partial\lambda_2}-\eta^2(\zeta_1+3\chi_2)\frac{\partial^3}{\partial{\lambda_1}^2\partial\lambda_2}\right]\gamma_2\\&+\left[\begin{matrix}\left(1+\dfrac{1}{\eta^2}\right)\chi_1+\dfrac{\partial^4}{\partial{\lambda_1}^4}+\chi_1\dfrac{\partial^4}{\partial{\lambda_2}^4}+\\2\chi_1\dfrac{\partial^2}{\partial{\lambda_2}^2}+(2\zeta_1+4\chi_2)\dfrac{\partial^4}{\partial{\lambda_1}^2\partial{\lambda_2}^2}\end{matrix}\right]\\&\eta^2\gamma_3+\frac{\hat{N}}{\Omega}(1-(e_0a)^2\nabla^2)\frac{\partial^2\gamma_3}{\partial{\lambda_1}^2}+(1-(e_0a)^2\nabla^2)\frac{R^2P}{\Omega}\\&=0\end{aligned}\tag{3}$$

where $P=-K_mw$ by Winkler model. The negative mark demonstrates that the direction of pressure P is reverse to initial buckling of the MTs, K_m denotes elastic constant of medium. Here the boundary conditions are simply supported.

2.2 The buckling solution of embedded microtubules

The buckling solution for simply supported boundary conditions is

$$\begin{aligned}\gamma_1(\lambda_1,\lambda_2,t)&=A_me^{i\omega t}\delta'(\lambda_1)\,cos(n\lambda_2)\\\gamma_2(\lambda_1,\lambda_2,t)&=B_me^{i\omega t}\delta''(\lambda_1)\,sin(n\lambda_2)\\\gamma_3(\lambda_1,\lambda_2,t)&=C_me^{i\omega t}\delta''(\lambda_1)\,cos(n\lambda_2)\end{aligned}\tag{4}$$

On putting (4) in (1)-(3), the following equations are obtained,

$$\begin{aligned}&\left\{\begin{matrix}-(\eta^2+1)\chi_2n^2\delta(\lambda_1)\\-\left[-1+\hat{N}\dfrac{(1-e_0a)^2\nabla^2}{\Omega}\right]\dfrac{d^2\gamma_1}{d{\lambda_1}^2}\end{matrix}\right\}A_m\\&+\left\{(\zeta_1+\chi_2)n\frac{d\gamma_2}{d\gamma_1}\right\}B_m+\\&\left\{\zeta_1\frac{d\gamma_2}{d\gamma_1}+\eta^2\left(-\chi_2n^2\frac{d\gamma_3}{d\lambda_1}-\frac{d^3\gamma_3}{d{\lambda_1}^3}\right)\right\}C_m=0\end{aligned}\tag{5}$$

$$\begin{aligned}&\left[-(\zeta_1+\chi_2)n\frac{d\gamma_1}{d\lambda_1}\right]A_m\\&+\left[\begin{matrix}\chi_2(1+3\eta^2)\dfrac{d^2\gamma_2}{d{\lambda_1}^2}\\-\dfrac{\hat{N}}{\Omega}((1-e_0a)^2\nabla^2)\dfrac{d^2\gamma_2}{d{\lambda_1}^2}-\chi_1n^2\delta''(\lambda_1)\end{matrix}\right]B_m\\&+\left[-\chi_1n\delta'''(\lambda_1)+\eta^2(\zeta_1+3\chi_2)n\frac{d^2\gamma_3}{d{\lambda_1}^2}\right]C_m=0\end{aligned}\tag{6}$$

$$\begin{aligned}&\left[\zeta_1\frac{d\gamma_1}{d\lambda_1}-\eta^2\left(\frac{d^3\gamma_1}{d{\lambda_1}^3}+\chi_2n^2\frac{d\gamma_1}{d\lambda_1}\right)\right]A_m\\&+\left[\chi_1n\delta''(\lambda_1)-\eta^2(\zeta_1+3\chi_2)n\frac{d^2\gamma_2}{d{\lambda_1}^2}\right]B_m\\&+\left[\begin{matrix}\left(1+\dfrac{1}{\eta^2}\right)\chi_1\gamma_3+\dfrac{d^4\gamma_3}{d{\lambda_1}^4}+\chi_1n^4\delta'''(\lambda_1)\\-2\chi_1n^2\delta'''(\lambda_1)-(2\zeta_1+4\chi_2)n^2\dfrac{d^2\gamma_3}{d{\lambda_1}^2}\end{matrix}\right]\\&\eta^2C_m+\frac{\hat{N}}{\Omega}(1-(e_0a)^2\nabla^2)\frac{d^2\gamma_3}{d{\lambda_1}^2}C_m\\&+(1-(e_0a)^2\nabla^2)\frac{R^2P}{\Omega}=0\end{aligned}\tag{7}$$

where $\varsigma=1+\left(\frac{e_0a}{R}\right)^2(n^2+\chi^2)$, and$\varpi=\frac{\hat{N}}{\Omega}$

This is homogeneous system of linear equations, therefore in matrix form the above system can be written as,

$$\left[E^{(2)}(n,\frac{L}{mR}\right]_{3\times3}\begin{bmatrix}\delta'\\\delta''\\\delta'''\end{bmatrix}=\begin{bmatrix}0\\0\\0\end{bmatrix}\tag{8}$$

For nontrivial solution,

$$det\left[E^{(2)}(n,\frac{L}{mR}\right]=0\tag{9}$$

3. Results and discussion

Fig. 1 is referred to the case when $e_0a=20\,nm$, circumferential wave number $n=2$ and longitudinal wave number, $m=2$. The graph is plotted between buckling load and dimensionless axial wavelength L/mR. In this graph the curves are compared for free and embedded MTs. For both the cases, with the increase in L/mR, the critical load for buckling first increases rapidly and after reaching a certain value it falls down. For very large values of L/mR, the buckling load tends to zero. This shows that when L/mR is very large then MTs buckle without any external load. This result confirmed the experimental findings. The

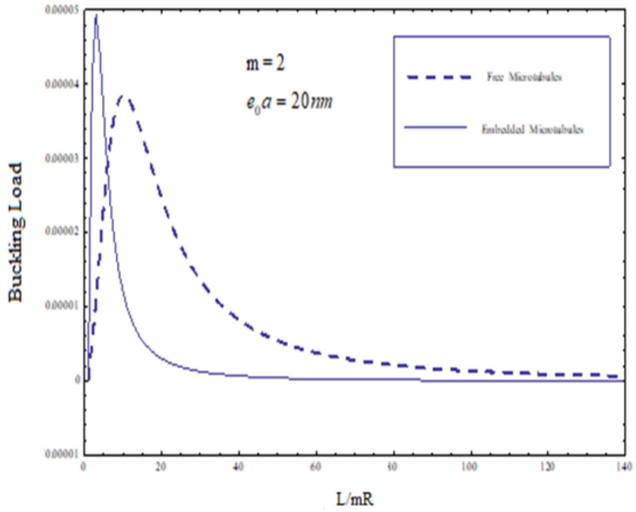

Fig. 1 Comparison of buckling loads between free microtubules and embedded microtubules for $m = 2$ plotted against L/mR

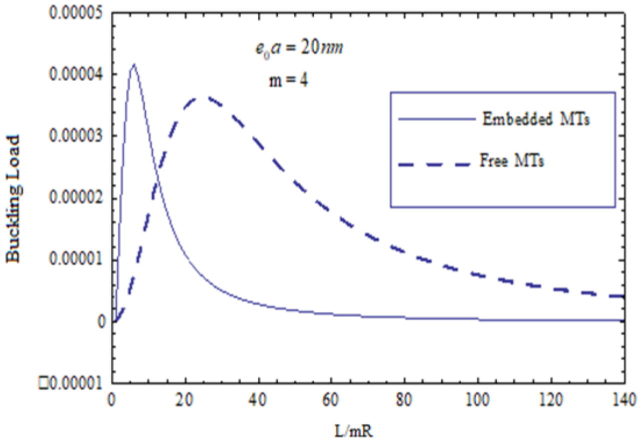

Fig. 2 Comparison of buckling loads between free microtubules and embedded microtubules for $m = 4$ plotted against L/mR

maximum value of critical load for free MTs is lesser than the maximum value of critical load for embedded MTs. It is due to the fact that, when MTs are embedded in an elastic medium the buckling is reduced or the load is increased. For embedded MTs, the buckling is lesser because the surrounding elastic matrix gives strength to the MTs.

The buckling load varies with the dimensionless axial wavelength *L/mR* with various longitudinal semi wave numbers, as shown in Fig. 2. As the dimensionless axial wavelength grows for each curve for fix m, the buckling load increases initially, achieves its maximum value, and subsequently drops, as illustrated in this figure for m here e_oa = 20 nm. As the buckling load grows in meters, the dimensionless axial wavelength corresponding to the minimum value is observed. The buckling load and the dimensionless axial wavelength *L/mR* are depicted on the graph. For both the cases, with the increase in L/mR, the critical load for buckling first increases rapidly and after reaching a certain value it falls down. For very large values of L/mR, the buckling load tends to zero. This shows that

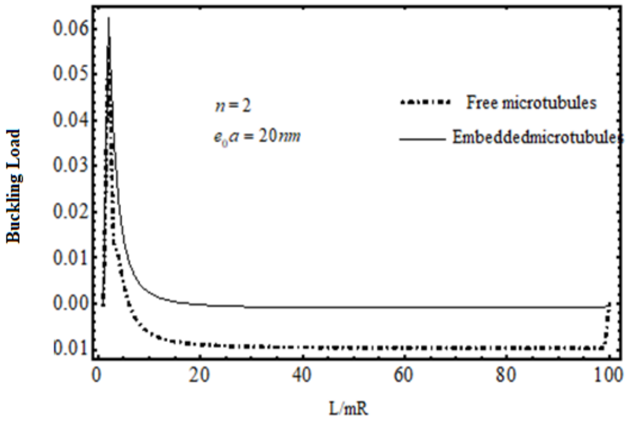

Fig. 3 Comparison of buckling loads between free microtubules and embedded microtubules for $n = 2$ plotted against L/mR

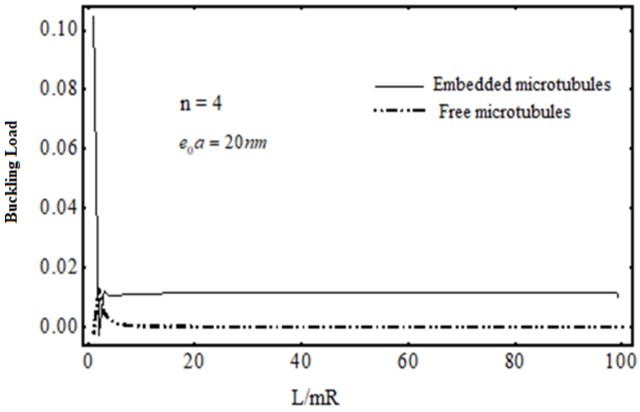

Fig. 4 Comparison of buckling loads between free micr otubules and embedded microtubules for $n = 4$ plotted against L/mR

when L/mR is very large then MTs buckle without any external load. This result confirmed the experimental findings. The maximum value of critical load for free MTs is lesser than the maximum value of critical load for embedded MTs. It is due to the fact that, when MTs are embedded in elastic medium the buckling is reduced or the load is increased. For embedded MTs, the buckling is lesser because the surrounding elastic matrix gives strength to the MTs. The critical load of MTs buckling as a function of dimensionless axial wavelength *L/mR* in the presence of an elastic material surrounding it and other small scale characteristics is displayed in Fig. 3.

This figure shows that when $e_oa = 20\,nm$, circumferential wave number $n = 2$ curves of graph are compared for free and embedded MTs. For both the cases, with the increase in L/mR, the critical load for buckling first increases quickly and after reaching a certain value it falls down. For very large values of L/mR, the buckling load approaches to zero. This shows that when L/mR is very large then MTs buckle without any external load.

The influence of small scale effects was rather considerable, however the influence of filament network elasticity on the value of the critical load was not significant due to the small dimensionless wavelength, as shown in

Fig. 4. On the other hand, at the large dimensionless axial wavelength L/mR, where the influence of small scale effects was strong, the filament network elasticity began to have a major impact on the value of the buckling load. For the cases of free and embedded MTs, with the increase in L/mR the critical load for buckling first increases after a certain value it falls down. For very large values of L/mR, the buckling load approaches to zero in case of free MTs. The maximum value of critical load for free MTs is lesser than the maximum value of critical load for embedded MTs. It is due to the fact that, when MTs are embedded in elastic medium the buckling is reduced or the load is increased.

4. Conclusions

Nonlocal orthotropic elastic shell model and Winkler model are combined and established a new nonlocal Winkler-like model for the investigation of buckling of MTs lying in natural elastic surrounding. Comparison of buckling loads for microtubules against dimensionless axial wavelength is done. It is observed that the buckling is either decreased or increased when MTs are immersed in an elastic media. Because the embedded MTs are strengthened by the surrounding elastic matrix, there is less buckling. Along with other small scale features, the critical load of MTs buckling in the presence of an elastic material surrounding it is shown as a function of dimensionless axial wavelength. The current work may be useful in applying the finite element approach to the analysis of the Winkler's model with embedded microtubules.

Acknowledgement

The authors extend their appreciation to the Deanship of Research and Graduate Studies at King Khalid University for funding this work through Large Research Project under grant number RGP2/95/45.

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