Mini Review

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Vibration of protein microtubules via scale-dependent continuum models

Abstract

Increasing the level of knowledge on the mechanics of biological structures such as protein microtubules is important because of two main reasons. The first reason is that the biological properties of living organisms are highly affected by their mechanical properties such as their elasticity modulus and resonance natural frequencies. Secondly, the mechanical properties and characteristics can be used as a clue in order to analyze the performance and functionality of a living organism. In this paper, the pioneering research studies on the vibrational behavior of protein microtubules as an important part of the cytoplasm are reviewed. Two widely used theoretical approaches, namely the pure nonlocal and nonlocal strain gradient models, are proposed. The natural frequencies of microtubules are strongly influenced by the stress nonlocality and the half wave number along the axial direction.

Keywords: protein microtubules, elasticity-based modelling, vibrational response, nonlocal elasticity, strain gradient

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Introduction

The mechanical behavior of biodegradable nanoscale/microscale materials[1–3] and natural ultrasmall biological structures such as protein microtubules (MTs)[4] have attracted considerable attention in scientific communities due to their promising functions in microelectromechanical systems[5–8] and living organisms,[9–11] respectively. One of the most important part of a living cell is MTs, which have many crucial roles to play in many cellular processes such as protein transportation and cell division. Analysing the mechanics of these cytoplasm components would help us to better understand many vital functions inside living cells. Various continuum-based models have been developed for the vibration of ultra-small materials in recent years.[12–15] Wang et al.[16] developed a classical shell theory in order to analyse the vibration of MTs; they used an orthotropic model since the shear and circumferential moduli of MTs are much lower than their axial modulus. In another work, Civalek and his co-workers[17] developed a non-classical beam model for the free oscillation of these cytoplasm components via application of the Eringen model of stress nonlocality; they captured size effects in their model since the dimensional vibration characteristics of a structure is a function of its size at microscale levels. Xiang and Liew[18] also proposed an atomistic-continuum model for the vibrational response of MTs incorporating the influence of boundary conditions; a mesh-free scheme is utilized for the vibration analysis as it exhibits intrinsic nonlocal properties. Farajpour et al.[19] developed a surface elasticity-based model to predict the mechanics of MTs in living cells; they concluded that surface effects are of noticeable importance in the accurate modelling of protein MTs. Moreover, Demir & Civalek[20] used a nonlocal modelling approach to investigate the deformation of protein MTs subjected to a concentrated force. In another interesting work, the application of a piezoelectric microscale layer in the smart control of MTs has been investigated via a scale-dependent shell model.[21]

More specifically, Beni & Zeverdejani[22] developed a scale-dependent shell model for analysing the MT vibrational behavior; they employed a modified model of the couple stress theory as a powerful tool to describe size dependency at microscale levels. In another research paper, Heireche et al.[23] investigated size influences on the vibrational behavior of MTs modeled via a nonlocal Timoshenko theory of beams. Li and his co-workers[24] analyzed the three-dimensional vibrational response of these living structures by developing a theoretical model based on the molecular structural mechanics. Moreover, Farajpour & Rastgoo[25] have analyzed the influence of added carbon nanotubes on the mechanical instability of a system of multiple MTs using a refined scale-dependent modelling. More recently, Taj et al.[26] have developed a shell model incorporating stress nonlocality for the vibration of MTs; they took into account orthotropic elastic properties for the protein MT in the shell model. In addition, a scale-dependent model has been developed in the literature to study the effect of taxol, a well-known stabilizing agent, on the mechanical stability of MTs.[27] In this paper, a brief review is performed on the available works on the vibrational response of MTs via utilizing scale-dependent elasticity-based modelling.

Scale-dependent modeling of MTs

In Fig. 1, the structure of a single MT is shown. MTs are rigid cylindrical filaments inside living cells, which are composed of two main tubulin types: 1) alpha type, and 2) beta type. Since the diameter of protein MTs is in the range of several nanometers, the nonlocal elasticity theory.[28–34] can be utilized as an appropriate theoretical tool for the vibrational analysis of these cytoplasm components. According to this size-dependent theory, the MT constitutive equation is mathematically described as:

$$\left[1-\left(e_0 a\right)^2 \nabla^2\right]\sigma_{ij}^{nl} = C_{ijkl}\varepsilon_{kl}, \qquad (1)$$

where e_0 is a constant coefficient used to calibrate the model.[35–37] This coefficient is calculated by comparing the results of the continuum-based simulation with those of experimental measurements or molecular dynamics. a is a characteristics length associated with the internal molecular configuration of the protein MT. For instance, this parameter can be set to an internal bond length. ε_{kl}, C_{ijkl} and σ_{ij}^{nl} denote the MT strain, elastic coefficients and nonlocal stress,

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respectively. In the above equation, ∇^2 is a mathematical operator, which is defined by the following relation for the nonlocal beam-based modelling of protein MTs

$$\nabla^2 = \frac{\partial^2}{\partial x^2}, \tag{2}$$

Here x is the axial coordinate. For MT nonlocal shell models, the mathematical operator ∇^2 is also expressed as

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{1}{R^2}\frac{\partial^2}{\partial \theta^2}, \tag{3}$$

where θ and R are the circumferential coordinate and the average MT radius, respectively (Figure 1). In addition to the nonlocal elasticity-based modelling, a refined continuum-based modelling has been proposed for the vibration analysis of ultrasmall materials such as graphene sheets, carbon nanotubes, and protein MTs. This refined modelling is established by Lim et al.[38] in 2015 via utilising the nonlocal and strain gradient theories. Based on this modelling, the modified constitutive equation of MTs is:

$$\left[1-(e_1 a)^2\nabla^2\right]\left[1-(e_0 a)^2\nabla^2\right]\sigma_{ij}^t =$$
$$\left\{1-(e_1 a)^2\nabla^2 - \ell_s^2\left[1-(e_0 a)^2\nabla^2\right]\nabla^2\right\}C_{ijkl}\varepsilon_{kl}, \tag{4}$$

where e_0, e_1 and ℓ_s represent the lower-order calibration coefficient, higher-order calibration coefficient and strain gradient parameter, respectively. Since this type of continuum modeling incorporates more scale parameters, it can better describe the size dependency at microscale levels. However, the computational cost of the modeling would significantly increase compared to the classical nonlocal modelling of protein MTs. The influence of the nonlocal parameter on the frequencies of a MT controlled by a piezoelectric nanoshell is depicted in Figure 2 for various half wave numbers in the axial direction. For more information about the mechanical properties of this system, an interested reader is referred to Ref.[21] From Figure 2, it is seen that the stress nonlocality in the constitutive relation of protein MTs leads to a significant reduction in the system frequency. This conclusion is based on the fact that the structure stiffness of MTs has a decreasing relation with the nonlocal parameter. Furthermore, it is noticeable that the influence of stress nonlocality is more significant at higher wave numbers.

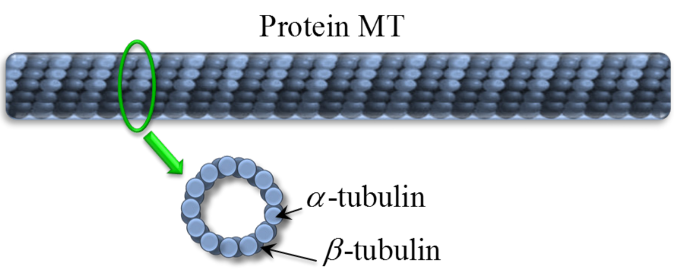

Figure 1 A protein MT composed of alpha and beta tubulins.

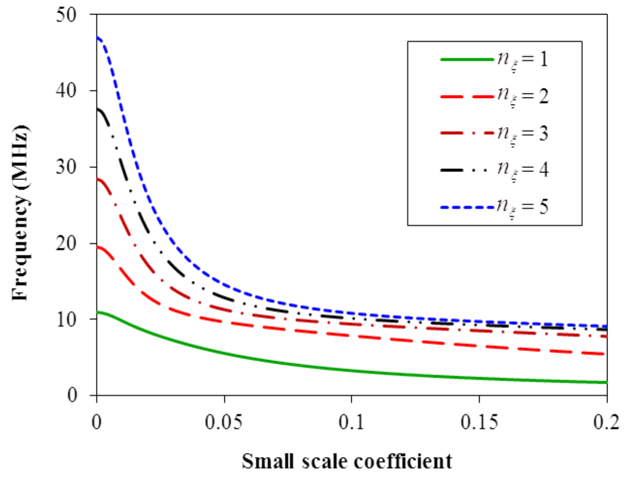

Figure 2 Frequency of MTs controlled by a piezoelectric nanoshell for various half wave numbers [21]; reproduced by permission from Elsevier.

Conclusion

In this article, a number of important research works on the vibration of protein MTs have been reviewed and discussed briefly. The main focus was on the scale-dependent elasticity-based modelling of the vibrational behavior of MTs. The proposed constitutive equations of MTs using the pure nonlocal elasticity and nonlocal strain gradient elasticity were elaborated. The influences of stress nonlocality and axial half wave number on the MT vibration were discussed. As the stress nonlocality enhances, the protein MT undergoes lower resonance frequencies. In addition, the stress nonlocality influence is more pronounced when the half wave number along the axial direction of the MT is increased. The stress nonlocality influence is strongly related to a significant decrease in the MT structural stiffness.

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Conflicts of interest

The author declares that there is no conflict of interest.

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