Composite Structures 127 (2015) 224–230

Contents lists available at ScienceDirect

Composite Structures

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

Analysis of macromolecular microtubules using the potential-based matrix displacement method

Ping Xiang [a,b], L.W. Zhang [c,*], K.M. Liew [a,b]

[a] Department of Architecture and Civil Engineering, City University of Hong Kong, Kowloon, Hong Kong Special Administrative Region
[b] City University of Hong Kong Shenzhen Research Institute Building, Shenzhen Hi-Tech Industrial Park, Nanshan District, Shenzhen, China
[c] College of Information Technology, Shanghai Ocean University, Shanghai 201306, China

ARTICLE INFO

Article history:
Available online 14 March 2015

Keywords:
Microtubules
Potential energy
Matrix displacement approach
Vibration behavior

ABSTRACT

This work presents an efficient matrix displacement approach for simulation of microtubules, a typical polyatomic macromolecular bio-structure in eukaryotic cells. The microtubule is modeled as an interatomic potential-based mechanical system. Unlike most of the continuum-based methods, the description of material properties in this model is based on fictitious bond and the interatomic potential energy is considered as based on the atomic force integral between basic macromolecule components. Meanwhile, superior to the conventional atomic-based simulation, the equilibrium state is solved in an efficient matrix framework comparable to the continuum-based structural mechanics approach. Following this approach, free vibration behavior of microtubules is intensively investigated. Microtubules with different boundary restrictions are considered in case studies and vibration modes and frequencies are obtained and compared with available references. It is found that the proposed macromolecular model performs with both accuracy and efficiency, and is superior to the two simulation regimes in atomic scale and continuum level.

1. Introduction

There are three types of filamentous polymers, microtubules, microfilaments and intermediate filaments that commonly exist in the cell cytoskeleton. Researchers are interested in exploring the mechanical aspects of cell functions by considering these components in eukaryotes. Among them, microtubules, described as cellular scaffolding, have been paid increasing in a wide range of research disciplines. The microtubule is a typical kind of polyatomic bio-structure composed of protein monomers, which is the most rigid filament and provides high mechanical strength to support and maintain cell shape. Other functions of cells, such as cell division and intracellular transport, are dependent upon the functions of microtubules. A comprehensive understanding of structural properties of microtubules is important for further development of biomechanics. However, the microtubule has an intricate build-up of different types of chemical elements. Millions or even billions of atoms cause great difficulties in implementing conventional atomistic simulations. Meanwhile, continuum mechanical modeling does not contain atomic scale information. Further efforts are needed for achieving a fundamental understanding of mechanics of microtubules.

For a long time, experimental tests have been used as a major tool in microtubule research. Structure morphology and responses of microtubules under simple loading tests have been captured in the past. Elastic properties were measured, but results have been scattered and have lacked consistency because of limitations of measurements and operations in small scales. Though advanced facilities and equipments were used, delicate stress, strain and sublet deformation behaviors still remain mysterious under laboratory conditions. Theoretical attempts have supplemented the efforts to address the limitations in practice. Various kinds of simulation methods have been adopted for exploring mechanical performance of nano and micro structures [1–8]. Atomistic simulations have been employed by Saini and Kumar [9] for investigating torsional deformation behavior of cracked gold nano-wires. He and Huang [10] presented an atomistic-based simulation of carbon nanotubes by using a cellular automata algorithm to improve the computing efficiency because conventional atomistic-based methods have computational limitations, such as molecular dynamics (MD). Existing MD approaches toward microtubules always focus on proteins and it is very hard to involve the overall performance of the whole microtubule structure [11–13]. Various continuum

* Corresponding author.
E-mail address: lwzhang@shou.edu.cn (L.W. Zhang).

http://dx.doi.org/10.1016/j.compstruct.2015.03.004
0263-8223/

mechanical approaches, including classical beam model, shell model and nonlinear and viscoelastic model have also been adopted for investigation of microtubules and other nano and micro structures [4,14–22]. He et al. [23] employed a continuum model accounting for van der Waals interaction for buckling analysis of multi-walled carbon nanotubes. Hu et al. [24] developed a nonlocal shell model for elastic wave propagation in single- and double-walled carbon nanotubes. Adali [25] proposed a variational principle for the study of microtubules based on the nonlocal orthotropic shell model. Wang et al. [26] developed a quasi-continuum approach based on the higher order Cauchy–Born rule. Based on nonlocal continuum and nonlocal discrete models, Demir and Civalek [27,28] studied torsional and longitudinal frequency and wave response of microtubules. Akgoz and Civalek [29] presented a free vibration analysis of single-layered graphene sheets in an elastic matrix by using a modified couple stress theory, and they also studied longitudinal vibration behaviors of microbars based on the strain gradient elasticity theory [30]. A modified strain gradient theory has also been employed by Zeverdejani and Beni [31] for vibration analysis of protein microtubules. Farajpour et al. [32] employed a modified Timoshenko beam model and further investigated surface effects on the buckling characteristics of microtubule systems in viscoelastic surrounding cytoplasm. Mahmoudinezhad et al. [33] presented a spring-mass model for vibration analysis of single-walled carbon nanotubes. Jin and Ru [34] studied the localized vibration of a microtubule surrounded by randomly distributed cross linkers. Chen et al. [35] investigated the influence of surface effects on coupling vibration of bioliquid-filled microtubules. The continuum mechanical models do not incorporate atomic interactions and special lattice structures information in small scales. Another alternative approach to bridge the gaps between conventional continuum and atomistic simulation is the atomistic-continuum approach, which involves atomic information and can overcome computational limitations for modeling the mechanics and physics of microstructures [36–40]. Havelka et al. [41] presented a semi-classical coarse-grained model for the electro-acoustic behavior of the mitotic spindle. Recently, atomistic-continuum theory has been developed for investigations of nano and micro scale lattice and crystal structures. By employing the meshfree method [42–46], Liew and Sun [2,3,47–49] have proposed an atomistic-continuum model and have further developed a systematic strategy to combine with meshfree method by using a higher order Cauchy–Born rule [2,3,47,48,50–52]. He et al. [53] and Wang et al. [54] have presented theories to consider the van der Waals interaction in continuum mechanics for study of multi-layered graphene and multi-walled carbon nanotubes. In this work a matrix displacement approach embedded with interatomic macromolecular model is proposed. Material properties of this approach are based on intrinsic atomic potential energy. A computational program is developed for modeling and simulating free vibration characterizations of microtubules. The developed method is expected to provide a fundamental understanding of macromolecular microtubules.

This paper is structured as follows. In Section 2, macromolecular potential energy in microtubules is evaluated by employing a homogenization technique. In Section 3, a matrix displacement method is developed based on interatomic potential for investigation of mechanical properties of microtubules; methodology used for numerical examination is presented. Based on the developed potential energy and matrix displacement method, study of free vibration behaviors of microtubules is presented in Section 4; predictions of vibration characteristics and biomechanical response of microtubules under various situations are captured by in-house programming and computing. Conclusions and discussions on this research are given in Section 5.

2. Description of potential energy in microtubules

Understanding material properties of microtubules is one of the preconditions to investigation of microtubule mechanics. Obviously, a conventional continuum model is not quite applicable for modeling the microtubules because morphology observations show that due to the spheroid shape of the tubulin monomer, deep holes and grooves exist on microtubule surface. Meanwhile, an exact consideration of the whole microtubule at atomic level is impractical and involves substantial computation. It is an alternate way to build an interatomic potential-based model by considering intrinsic atomic interaction, for modeling the mechanical properties of microtubules. To develop a small scale interatomic potential-based model, it is vital to find a way to describe material properties of the nano or micro structure based on its inherent potential energy. The microtubule is made up of the basic subunit components, tubulin heterodimers, made of two types of tubulin proteins, α-tubulin and β-tubulin. Though these two kinds of tubulins are differently named and there are some subtle differences in their atomic structures, they have nearly the same mechanical interaction as the neighboring tubulin monomers because they have similar atomic components. The protofilament is formed by tubulin heterodimers arrayed in a line in longitudinal direction. Normally, the microtubules can be viewed as hollow cylindrical tubes formed by 13 protofilaments gathered circumferentially (Fig. 1). Tubulins are macromolecular proteins, which are self-rigid bodies under loading actions. Non-covalent interaction causes the mutual actions and reactions between tubulin heterodimers, though covalent bonds also exist inside bodies of protein themselves. Cornell et al. [55] reported mutual potential energy between pairs of atoms for proteins and grounded on this an atomistic-continuum mechanical approach is formulated on the basis of the proposed homogenization technique to determine interatomic potential between tubulin monomers [36–40]. Fictitious bonds are proposed for consideration of the interatomic potential energy and deformation between tubulin proteins.

In order to establish a reliable model for defining mechanical properties of microtubules, it is of great importance to precisely evaluate the potential energy of the fictitious bond, which stands

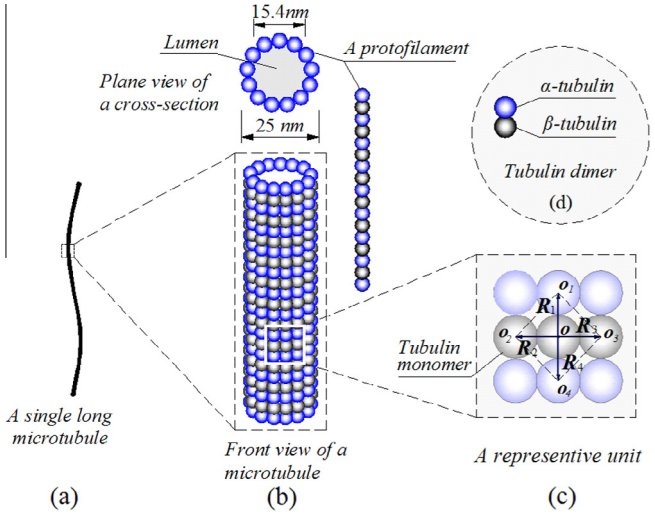

Fig. 1. Formation of the interatomic-potential based model of a microtubule: (a) single long microtubule; (b) cross-section and front view of the structure of a microtubule and its subunits; (c) representative unit cell of the energy homogenized model of polyatomic microtubule structure, tubulin monomers are modeled as spatial spheroids; and (d) dimeric structure of a tubulin dimer made up of a pair of α- and β-tubulins from the microtubule.