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Meshfree simulation of temperature effects on the mechanical behaviors of microtubules

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ABSTRACT

The temperature-related mechanical behaviors of microtubules are investigated by way of the developed meshfree computational framework. An atomistic-continuum constitutive relationship is formulated for bridging-scale simulations of microtubules from polyatomic structure to continuum meshfree modeling. The establishment of a specific meshfree theory is based on high-order gradient continuity, by incorporating a higher-order Cauchy–Born rule. The influence of temperature on the critical buckling force and free vibration frequencies of microtubules is intensively studied. It is realized from the simulation results that temperature significantly affects the mechanical behaviors of microtubules. The critical buckling force and natural vibration frequencies of microtubules decrease with increases in temperature. A lower temperature will always result in a higher flexural rigidity, thus benefiting the mechanical strength of microtubules. In contrast, an elevated temperature will have negative impacts on microtubule stiffness. Microtubules with typical boundary restrictions subjected to different temperatures are included in the analysis. A series of simulation results on the critical buckling force and natural vibration frequencies of microtubules covering a wide range of microtubule lengths is presented for the purpose of the provision of engineering references.

1. Introduction

Three major kinds of filament exist within the cytoskeleton – the microtubule, microfilament and intermediate filament – of which the microtubule is the most rigid. The mechanical behaviors of microtubules have been investigated in recent decades because of their importance to the biomechanical functions of the cytoskeleton within the context of eukaryotic cells [1–4]. The microtubule provides the main mechanical strength by which to maintain the cell shape and afford intracellular transportation and exchanges of organelles. The microtubule structure has the appearance of a cylindrical hollow tube composed of circumferentially gathered protofilaments.

It is understood that the mechanical behaviors of microtubules are sensitive to environmental conditions, such as the elastic or viscoelastic medium and temperature. Experiments have been conducted in order to investigate the temperature-dependent rigidity of microtubules. It is reported that the measured flexural rigidity of taxol-free microtubules decreases as temperature increases. Elevated temperatures will ultimately decrease flexural rigidity by one half, when the temperature is increased from 20 °C to 35 °C. Data on the flexural rigidity of microtubules with lengths ranging from 8 μm to 12 μm under temperature environments ranging from 20 °C to 35 °C have been obtained in these experimental studies. Thus, it is deducible that temperature also significantly influences such mechanical characterizations as the critical buckling force and natural vibration frequencies of microtubules. However, reports on the simulation of the temperature-dependent mechanical behaviors of microtubules are scarce.

As experiments can take only very limited measurements of test samples, so the result values from tests are also limited. Therefore, it is meaningful to further study the critical buckling behaviors and vibration characterizations of microtubules via computational mechanical approaches by considering temperature influences.

In order to study nano- and micro-structures, various approaches have been developed, mainly consisting of atomistic simulations, continuum mechanical modeling and multiscale methods. These three methods have their own specific advantages and disadvantages. Atomistic simulation ensures an accurate calculation of the force field between each pair of atoms involved in

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the consideration; however, the computational cost is very high, especially in the case of polyatomic structures such as the microtubule. A single long microtubule is composed of billions of different types of atoms that it is impossible to consider using traditional atomistic simulation approaches. Continuum mechanical simulation methods are developed for the modeling of materials and structures in small-scale, although the continuum constitutive relationship does not involve atomic scale interactions.

Intrinsic size effects are not deflected in the formulation of continuum mechanics. Additional efforts have been made to further modify conventional continuum theory by taking into consideration the interatomic potentials of micro- and nano-structures. However, the methods of implementation remain indirect, and it is not possible to consider nanoscale lattice structures with the continuum model. In order to implement continuum mechanical modeling, the finite element method (FEM) has been developed with different types of models, including beam, plate and shell models, for use in the place of theoretical mechanical analysis, for the provision of numerical solutions to complex problems in engineering.

Many works of research have been founded on atomistic simulations, nano mechanics and FEM research, which are invaluable to the development of the theoretical basis of this research [5–10]. By employing atomistic simulation, the torsional deformation of cracked gold nano-wires has been investigated by Saini and Kumar [11]. Continuum plate and shell theory has been developed [12,13] and applied to nano mechanics, with appropriate modifications. Shen [14–16] proposed a nonlocal deformable shell model and published a series of works on the study of the nonlinear vibration and bending, buckling and post-buckling of microtubules with a consideration of axial compression force and elastic medium environments. Wang et al. [2,17] employed the orthotropic elastic shell model to investigate the buckling behaviors and vibration behaviors of microtubules. Wang et al. [18] and Wang and Zhang [19] further investigated the dynamic behaviors of microtubules embedded in cytosol and their circumferential vibration performances with long axial wave lengths. Subsequently, Zhang and Wang [20] developed a structural mechanics model by taking into consideration configuration effects.

Civalek and Akgoz [3] and Civalek and Demir [21] developed a nonlocal Euler–Bernoulli beam theory to analyze the bending and free vibration behaviors of microtubules with different boundary conditions. Farajpour et al. [22] applied microtubule networks to living cells and studied the surface effects of their mechanical characteristics. Nonlocal continuum and nonlocal discrete models have been employed for the investigation of the torsional and longitudinal vibration behaviors and wave propagation problems of microtubules by Demir and Civalek [23] and Civalek et al. [24]. Akgoz and Civalek [25,26] presented studies on the mechanical behaviors of microtubules based on strain gradient elasticity and modified couple stress theories. The strain gradient theory has been adopted by Mustapha and Wong [27] specifically for torsional frequency analyses of microtubules with end attachments. A modified strain gradient theory has been employed by Zeverdejani and Beni [28] for a study of the nano scale vibration of protein microtubules.

Recently, Mahmoudinezhad et al. [29] studied the vibration behaviors of single-walled carbon nanotubes by way of a spring-mass model. Adali [30] employed the semi-inverse method and formulated the variational principle to investigate the buckling loads of microtubules based on the nonlocal orthotropic elastic shell model. Chen et al. [31] considered bioliquid-filled microtubules and conducted studies on their vibration behaviors. The coarse-grained model is also considered a feasible way in which to model polyatomic structures without the need to trace each individual atom, and this approach has already been applied to the mechanical research of polyatomic biostructures. Havelka et al. [32] reported on a study which employed a semi-classical coarse-grained model to investigate the electro-acoustic behaviors of the mitotic spindle.

The FEM approaches are typically restricted by elements, which results in many problems with the application of FEM to C^1 continuity problems. Point-based methods have been developed to make up for the deficiencies generated by elements [33–35] and which naturally satisfy the C^1 continuity [36–40]. Liew et al. [37] and Xiang and Liew [36,38–40] established a high-order deformation gradient continuum constitutive relationship for the prediction of the elastic properties of microtubules. Further, they developed an overall meshfree computational framework based on the atomistic-continuum and systematically investigated the mechanical behaviors of microtubules, including buckling analysis, vibration and dynamics. The development of an atomistic-continuum meshfree framework has been accomplished with the successful application of a higher-order Cauchy–Born rule [36–40], which is utilized to describe the deformation of fictitious bonds with high accuracy.

Zhang et al. [41] and Wang et al. [42] studied the elastic and mechanical behaviors of carbon nanotubes and the human erythrocyte membrane using the developed higher-order Cauchy–Born rule. It is proved in their works that the mapping efficiency of vectors can be substantially enhanced by including the higher order terms within the standard Cauchy–Born rule. Subsequently, Liew and Sun [43] further developed a meshfree higher-order gradient continuum theory by incorporating the higher-order Cauchy–Born rule, and successfully applied the theory to the mechanical analysis of single-walled carbon nanotubes. Later, an atomistic-continuum relationship and meshfree computational framework were developed for the prediction of the elastic properties and specific analysis of the overall mechanical behaviors of microtubules [36–40,44,45].

Simulation research into the temperature-related mechanical behaviors of microtubules remains insufficient and, inspired by this situation, the current work focuses on the mechanical behaviors of microtubules by considering the effects of environmental temperature. An atomistic-continuum constitutive relationship is developed and incorporated into a meshfree computational framework by including temperature effects. In the development of this meshfree mechanical simulation framework, the impact of temperature on the rigidity of microtubules is considered alongside experimental works [46,47]. Then, the temperature-related mechanical behaviors of microtubules, including critical buckling force and vibration frequencies, are explored by way of the developed atomistic-continuum meshfree framework.

This paper is organized as follows. Section 2 introduces the polyatomic structure of microtubules and an atomistic continuum constitutive model for meshfree mechanical analysis. Temperature influences on the potential energy of microtubules are included. Section 3 presents the detailed derivation and formulation steps of the meshfree computational framework for the calculation of the critical buckling force and free vibration behaviors of microtubules. The construction of shape functions in the meshfree analysis is based on the moving least square (MLS) approximation, which is also presented. Section 4 presents numerical studies of the mechanical behaviors of microtubules. Various case studies are conducted in order to fully understand the influence of temperature. Various boundaries and lengths are involved in the study of critical buckling force and vibration frequencies. The temperature-related mechanical behaviors of microtubules are intensively discussed and presented. Concluding remarks are made in Section 5.