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Nonlocal orthotropic shell model applied on wave propagation in microtubules

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ABSTRACT

Wave propagation in microtubules is investigated based on the nonlocal elastic theory. The complete analytical formulas of wave velocity are obtained, and the results demonstrate that the small scale effect can reduce the velocity, especially for large longitudinal wave-vector and large circumferential wave number. When the wave length is smaller than 80 nm, the small scale effects are more significant. The results match the conclusions of lattice vibration well. Besides, temperature is taken into account and the results show that the temperature effect on waves in microtubules is not monotonous but have a certain stableness in higher and lower temperature zone. The methods and results may also support the design and application of nano devices such as micro sound generator etc.

1. Introduction

Microtubules widely exist in eukaryotic cells and play many essential roles. A microtubule looks like a hollow cylinder (Fig. 1A) which is usually formed by 13 protofilaments consisted by $\alpha\beta$-tubulin dimers. As one of the three major components of cytoskeleton, microtubules have the maximum rigidity [1]. From the view of cell scale, microtubules help to shape the cell, keep the rigidity of cell, and act as an important part of cell's movement and deformation [2]. Intracellularly, they are the important paths for transportation of motor proteins, secretory vesicles, pigment granules and ions, During cell division, microtubules manipulate the chromosomes' movements, and distribute organelles and cytoskeletal proteins to each daughter cell [3,4].

Microtubules' functions are largely determined and regulated by their dynamical behaviors, for example, wave motions. The oscillation of microtubules can generate electric and magnetic fields in adjacent cytoplasm because of molecules' polarity [5], which is so important for intracellular deterministic motions [6] . Microtubules are basic parts of axons, and the knowledge of wave in microtubules is essential in understanding the injuries of brain tissues [7]. Daneshmand et al. [8] have summarized several cellar functions related to wave in microtubules: (1) Movement of macromolecule and organelle along microtubules; (2) External mechanical stimulation or internal thermal agitation; (3) Movement of cilia and flagella; (4) Growth of microtubules, etc.

To understand wave motions in microtubules, Qian et al. [2] firstly introduced the classical elastic shell model and obtained the wave velocity, and then the shear effects on wave were considered by Daneshmand et al. [8]. Recently, Tai and

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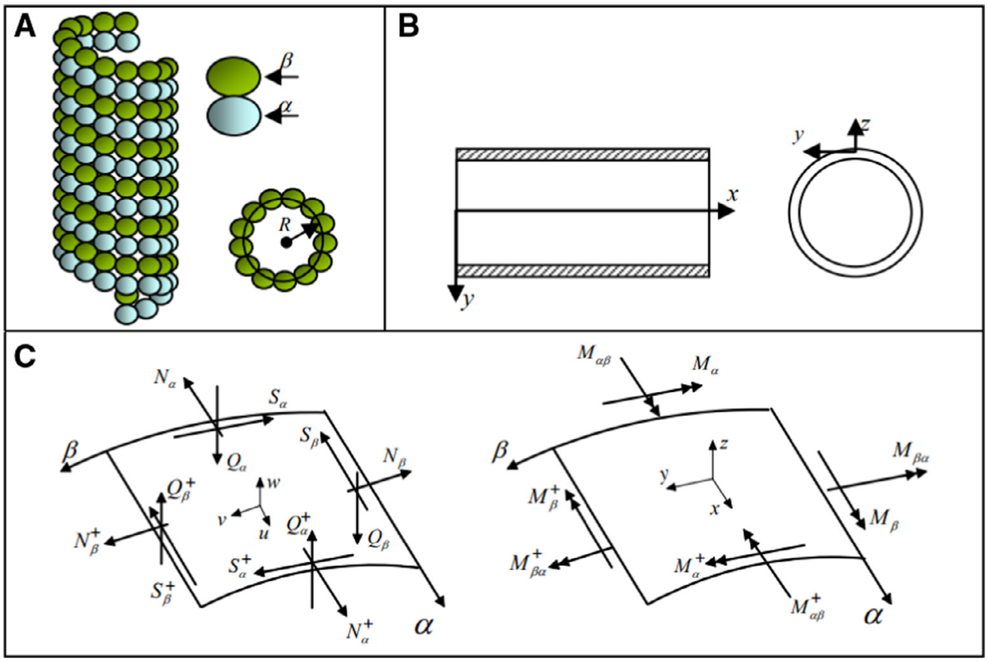

Fig. 1. Model of microtubules. (A) Configurations of a typical microtubule; (B) Coordinate system of microtubule; (C) Force analysis of shell element, where $F_{ij}^+ = F_{ij} + \frac{\partial F_{ij}}{\partial i} di$, $i = \alpha, \beta$, and $F$is generalized force.

Zhang [9] took the cytoplasm medium into account using Pasternak model, which predicted that the surrounding medium may remarkably increase the radial wave's velocity. However, it notes that microtubules are quite small. The effective radius R of a microtubule is about 12.8 nm (Fig. 1A). Generally, the length of microtubules is about several hundred nanometers. In such a small scale (micro/nano meters), the behaviors of structures are different from those of macro scale, which is the so called "small scale effects". When a wave is propagating in microtubules, the wavelength will be very small because of size limitation (The very long wavelength corresponds to the overall movement of a microtubule). Or in other words, the wave-vector is very large since it is inversely proportional to wavelength. Based on lattice dynamics theory [10], the waves with large wave-vector are dispersive and cannot be dealt with by the classical elastic models which use long wavelength assumption.

Though the scale of microtubules is quite small, at present we may find it is still very complex to simulate the microtubules from the level of atoms based on lattice dynamics. When it was used to predict microtubules' mechanical properties, the all-atom simulations may be not reliable sometimes [11,12] and the reasons partially lie in the difficulties of controlling the initial conditions and the calculating processes. But by introducing the small scale effects, some generalized continuum theories could describe the behaviors of micro/nano structures well.

Utilizing interpolation functions, the lattice dynamics theory can transit to nonlocal elastic theory [13]. The original idea of nonlocal elastic theory is the long range interaction between atoms/molecules such as Coulomb force, van der Waals force etc. Since long range interactions widely exist in the microscopic world, nonlocal elastic theory has a clear physical picture. Within nonlocal theory, the stress at a particular position is not only related to the local strain, but also related to long range interactions from the adjacent areas (This is the reason why the theory is named with "nonlocal"). What's more, the nonlocal elastic theory has a relatively simple mathematical expression. So the theory has been widely used on micro/nano structures including microtubules. Using nonlocal elastic theory, Gao and his partners [1,14,15] showed that the small scale effect may significantly change microtubules' persistence length which is a direct representation of microtubules' stiffness. The small scale effects also influence microtubules' buckling [1,14–18], postbuckling [17,18] and bending [19,20] . In addition, many researchers [20–23] were interested in microtubules' vibrations and indicated that the small scale effects have a notable impact on the dynamic properties of microtubules.

Motived by these ideas, we attempt to model the wave propagation in microtubules taking the small scale into account in the present work. At the early days of nonlocal theory, Eringen [24] had proved the theory can give a wave dispersion curve which is very close to the acoustic lattice vibration at whole Brillouin zone. So the nonlocal theory is applied in the paper. With nonlocal rod model, Demir and Civalek [25] had provided a primary results of the torsional and longitudinal waves in microtubules. But microtubule has a hollow cylinder structure, the shell model should be utilized if we want to learn more about waves in microtubules. Before the present work, researchers [26,27] have successfully applied nonlocal isotropic shell model on the wave propagation in carbon nanotube and the results showed satisfying accuracy. However, the nonlocal isotropic shell cannot be applied on microtubules directly because of anisotropy in microtubules. Experiments