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Predicting buckling behavior of microtubules based on an atomistic-continuum model

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ABSTRACT

An atomistic-continuum model is proposed for microtubules. A higher-order gradient continuum constitutive relationship is established, and elasticity and global buckling of microtubules are studied intensively. As a typical macromolecular bio-system, atomic components and structures are much more complicated. Traditional atomistic simulation methods and classical continuum approaches have their own fundamental drawbacks in dealing with this large atomic system. Adopting a homogenization technique, this paper proposes a concept of fictitious bonds for microtubules to link the large atomic structure with continuum description. After selecting a representative unit, the fictitious bond energy equals to the energy stored in the continuum model. The higher-order Cauchy–Born rule is used to approximate the deformation of fictitious bonds under arbitrary loading conditions. A mesh-free numerical scheme is specifically developed for modeling computation. The elastic modulus and critical compressive force are predicted. Representative case studies are presented, and some results are obtained and discussed.

1. Introduction

Microtubules are protein filaments that exist universally in eukaryotic cells. Together with microfilaments and intermediate filaments, they make up the whole cytoskeleton, which has specific biophysical functions and mechanical properties required for normal growth and maintaining the cell shape. The mechanical behavior of cytoskeleton is primarily governed by microtubules, the most rigid component of the cytoskeleton in eukaryotic cells (Alberts, 1994). For a long time, researchers have attempted to unfold its subtle mechanical properties and behavioral mechanism through various methods, including experimental tests and theoretical analyses, but have still been unable to find an efficient way to deal with this problem with sufficient efficiency and accuracy.

Microtubules are frequently subjected to pressure. Rod-like buckling occurs in many cases under critical pressure, under different boundary restrictions. In early years, laboratory tests served as major possible approaches to investigate the microtubule (Fygenson et al., 1997; Kurachi et al., 1995; Odde et al., 1999; Wang et al., 2001). The elastic properties and flexural rigidity have been experimentally investigated by direct measurement of buckling by some researchers (Gittes et al., 1992; Kurachi et al., 1995; Mizushimasugano et al., 1983; Venier et al., 1994). However, test results lack consistency to some degree and are scattered over a wide range. The measurements are difficult in nanoscale and may not accurately capture the mechanical properties of individual microtubules due to the need for very precise instruments and manipulation. Along with these experimental measurements, various theoretical attempts, including atomic-based methods and continuum methods, have also been made in theoretical studies (Jiang and Zhang, 2008; Li et al., 2006; Molodtsov et al., 2005; Qian et al., 2007; Wang et al., 2006a,b). Atomic-based methods, such as molecular static and dynamic, are capable of predicting various material mechanisms such as fracture, dislocation nucleation and propagation (Liew et al., 2004a,b; Liu et al., 2010). However, atomistic simulation depends much on computational resources, and it also has time and size limitations. In this sense, some continuum based methods have many advantages in dealing with large atomic structures (He et al., 2005; Lim, 2010; Wang et al., 2006a). However, conventional continuum based mechanical models do not contain fundamental atomic scale information. To study sufficiently long microtubules, the billions of atoms constitute a huge obstacle for traditional molecular dynamics (MD) approaches. At the same time, the conventional continuum mechanical model is unable to incorporate atomistic interaction within material properties and capture the microscale physical laws of nanostructures. Thus, it can only give one-sided descriptions of atomic structures.

Another alternative method that emerged for bridging the scale between atomic simulation and the continuum method is the atomistic-continuum method, which is a viable means of studying materials and systems with high efficiency and adequate accuracy. In atomistic-continuum method, material properties and

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