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BRIDGING-SCALE MODELING OF BIOMECHANICAL BEHAVIOR OF MICROTUBULES

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ABSTRACT

A computational modeling of the biomechanical behavior of microtubules is carried out. A single microtubule contains up to billions of different types of atoms. To analyze a microtubule, the challenge is to develop a practical theory to describe this kind of polyatomic structure with both result accuracy and computing efficiency. This work proposes a bridging-scale technique based on the intrinsic interatomic potential and a continuum description method, and hence the overall mechanical performance of microtubules could be studied. The work begins with evaluation of interatomic potential using a homogenization technique; large numbers of different types of atoms are replaced by a product of volume densities and the occupied space volumes. The potential energy stored between the basic subunit of microtubules and tubulin dimmers is obtained from a mutual definite integral process between pair bodies [1]. Without tracing every single atom, deformation of macromolecules components is determined by the proposed fictitious bond connecting central points of neighboring bodies. A mesh-free theoretical and numerical framework based on a higher-order Cauchy-Born rule under the higher-order gradients continuity has been specifically constructed [2]. This simulation scheme is generally applicable and can be employed to study the overall mechanical behavior of microtubules. With the proposed methodology, elastic properties, transverse and longitudinal buckling and post-buckling behaviors, vibration modes, natural frequencies and dynamic responses are numerically simulated.

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