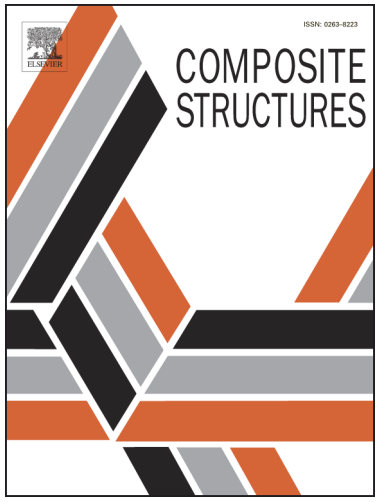

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A mesh-free computational framework for predicting vibration behaviors of microtubules in an elastic medium

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Abstract

An element-free computational framework is developed for the simulation of vibration characterizations of microtubules immersed in an elastic medium. The considered microtubules are of a typical polyatomic composite macromolecular bio-structure. Rather than observing each individual atom, the billions of atoms present within the microtubules are considered by way of a homogenization technique. The interatomic potential between tubulin monomers is first obtained from the atomic structure. By employing a higher-order Cauchy-Born rule, this interatomic potential is schematically introduced into a continuum counterpart for element-free numerical solutions based on higher-order deformation gradient continuity. The established simulation framework runs simultaneously on both the atomic scale and the continuum level. The free vibration behaviors of microtubules are analyzed in order to observe medium effects. It is found that the vibration frequencies of microtubules are generally increased by considering the effects of the surrounding environment. The frequency value increases with increased medium modulus as a result of the stiffening effect of the medium on the microtubule structure. However, this stiffening effect tends to reduce for higher frequency vibration modes. This work considers the polyatomic structure of microtubules in an atomistic-continuum manner, which has certain advantages over conventional continuum mechanics and atomistic simulation methods.

Keywords: microtubules; vibration behavior; elastic medium

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