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Analysis of microtubules based on third-order Cauchy-Born rule using element-free method

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Abstract

The Cauchy-Born rule is an efficient formula to schematically connect the deformation of atomic structures with a reciprocal continuum field. It is especially useful to the implantation of multiscale theories and has already been successfully applied in the mechanical modeling of microtubules. In atomistic-continuum approaches, the continuum description of material properties can be evaluated by minimizing potential energy of an atomic structure. Moreover, the intrinsic interatomic potential can be obtained at the microscopic atomic level and further embedded in a macroscopic continuum model using the Cauchy-Born rule. The conventional Cauchy–Born rule,however, is not accurate enough in numerical implementations, and the errors can be removed mostly by including higher-order terms based on Taylor series. This work aims to quantitatively evaluate the influences of higher-order terms on the modelling accuracy of the mechanical behaviors of microtubules. The first-, second- and third-order Cauchy-Born rules are developed for atomistic-continuum modelling. As the continuum mechanics implementation of the third-order Cauchy-Born rule requires C_2 continuity property, a specific mesh-free computational scheme based on third-order deformation gradient continuum is developed in order to suit the third-order Cauchy-Born rule for the mechanical simulation of microtubules. A series of simulation results are presented for the evaluation and discussion.

Keywords: higher-order Cauchy-Born rule; atomistic-continuum; higher-order deformation gradient continuum; mesh-free method; microtubules

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