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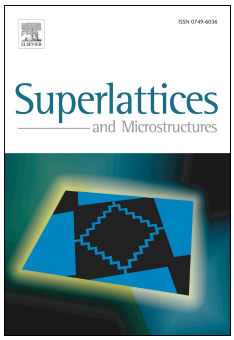

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Free vibration analysis of single-walled boron nitride nanotubes based on a computational mechanics framework

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Abstract

Free vibration behaviors of single-walled boron nitride nanotubes are investigated using a computational mechanics approach. Tersoff-Brenner potential is used to reflect atomic interaction between boron and nitrogen atoms. The higher-order Cauchy-Born rule is employed to establish the constitutive relationship for single-walled boron nitride nanotubes on the basis of higher-order gradient continuum theory. It bridges the gaps between the nanoscale lattice structures with a continuum body. A mesh-free modeling framework is constructed, using the moving Kriging interpolation which automatically satisfies the higher-order continuity, to implement numerical simulation in order to match the higher-order constitutive model. In comparison with conventional atomistic simulation methods, the established atomistic-continuum multi-scale approach possesses advantages in tackling atomic structures with high-accuracy and high-efficiency. Free vibration characteristics of single-walled boron nitride nanotubes with different boundary conditions, tube chiralities, lengths and radii are examined in case studies. In this research, it is pointed out that a critical radius exists for the evaluation of fundamental vibration frequencies of boron nitride nanotubes; opposite trends can be observed prior to and beyond the critical radius. Simulation results are presented and discussed.

Keywords: computational framework; single-walled boron nitride nanotubes; higher-order Cauchy-Born rule; free vibration behavior.

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