Jiang, Lai; Guo, Wanlin

Analytical solutions for elastic binary nanotubes of arbitrary chirality. (English)

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Summary: Analytical solutions for the elastic properties of a variety of binary nanotubes with arbitrary chirality are obtained through the study of systematic molecular mechanics. This molecular mechanics model is first extended to chiral binary nanotubes by introducing an additional out-of-plane inversion term into the so-called stick-spiral model, which results from the polar bonds and the buckling of binary graphitic crystals. The closed-form expressions for the longitudinal and circumferential Young's modulus and Poisson's ratio of chiral binary nanotubes are derived as functions of the tube diameter. The obtained inversion force constants are negative for all types of binary nanotubes, and the predicted tube stiffness is lower than that by the former stick-spiral model without consideration of the inversion term, reflecting the softening effect of the buckling on the elastic properties of binary nanotubes. The obtained properties are shown to be comparable to available density functional theory calculated results and to be chirality and size sensitive. The developed model and explicit solutions provide a systematic understanding of the mechanical performance of binary nanotubes consisting of III–V and II–VI group elements.

MSC:

74L15 Biomechanical solid mechanics

Keywords:

binary nanotubes; elastic properties; molecular mechanics; chirality; analytical solutions

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