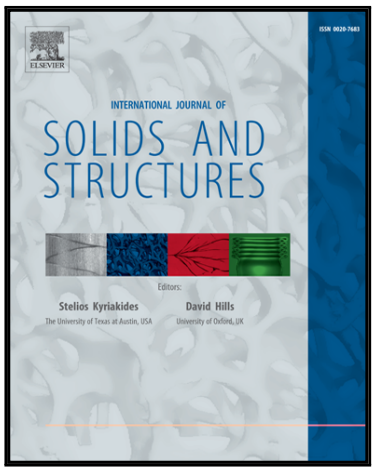

Radial deformation of single-walled carbon nanotubes adhered to solid substrates and variations of energy: atomistic simulations and continuum analysis

Xuebo Yuan , Youshan Wang

PII: S0020-7683(18)30176-8
DOI: 10.1016/j.ijsolstr.2018.04.021
Reference: SAS 9977

To appear in: *International Journal of Solids and Structures*

Received date: 13 February 2018
Revised date: 16 April 2018
Accepted date: 25 April 2018

Please cite this article as: Xuebo Yuan , Youshan Wang , Radial deformation of single-walled carbon nanotubes adhered to solid substrates and variations of energy: atomistic simulations and continuum analysis, *International Journal of Solids and Structures* (2018), doi: 10.1016/j.ijsolstr.2018.04.021

Radial deformation of single-walled carbon nanotubes adhered to solid substrates and variations of energy: atomistic simulations and continuum analysis

Xuebo Yuan, Youshan Wang*

Center for Composite Materials and Structures, Harbin Institute of Technology, Harbin, 150080, P.R. China

*To whom correspondence should be addressed: E-mail: wangys@hit.edu.cn

Acknowledgments

Xuebo Yuan is grateful to Mr. Zheng Liang for his help in MD simulations. Ms. Qiuqiu Fan and Dr. Fei Li are thanked for helpful discussions. This work was supported by the National Key Laboratory Fund of China [grant number 9140C490208130C49001].

Declaration of interest

Declarations of interest: none.

Abstract

Radial deformation of carbon nanotubes (CNTs) adhered to substrates can strongly influence their physical properties and the performance of CNT-based nanodevices. Here we explore the radial deformation and related energy variations of single-walled carbon nanotubes (SWCNTs) attached to solid substrates by adopting the classical molecular dynamics (MD) simulations and continuum analysis. The radial deformation of a SWCNT can be divided into three stages: the drop-shaped stage, the half-hourglass-shaped stage and the half-dumbbell-shaped stage. Three continuum models are established to mimic the radially deformed configurations.