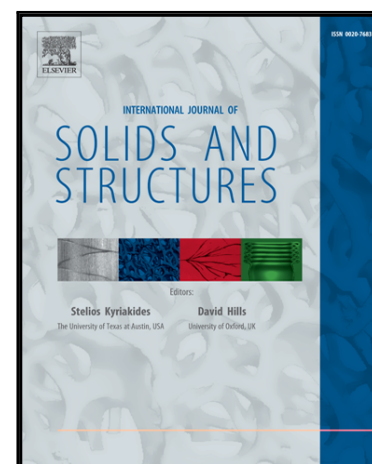


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# Radial deformation of single-walled carbon nanotubes adhered to solid substrates and variations of energy: atomistic simulations and continuum analysis

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## 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.

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