

**Carbon Nanotube Mechanics:
Continuum Model Development from Molecular Mechanics Virtual Experiments**

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ABSTRACT

Carbon Nanotubes (CNTs) hold great promise as an important engineering material for future applications. To fully exploit CNTs to their full potential, it is important to characterize their material response and ascertain their material properties. We have used molecular mechanics (MM) simulations to conduct virtual experiments on single-wall and multi-wall carbon nanotubes (SWNTs and MWNTs respectively) similar to those performed in the mechanics of materials laboratory on a continuum structure. The output (energy and deformation rather than the load and deflection) is used to understand the material response and formulate macroscopic constitutive relations.

From results of MM simulations of axial and torsional deformations on SWNTs, Young's modulus, the shear modulus and the wall thickness of an equivalent continuum tube made of a linear elastic isotropic material were found. These values were used to compare the response of the continuum tube, modeled as an Euler-Bernoulli beam, in bending and buckling with those obtained from the MM simulations.

MM simulations have been carried out to find energetically favorable double-walled carbon nanotube (DWNT) configurations, and analyze their responses to extensional, torsional, radial expansion/contraction, bending, and buckling deformations. Loads were applied either to one wall or simultaneously to both walls of an open-ended DWNT. These results were compared against SWNT results. It was found that for simple tension and torsional deformations, results for a DWNT can be derived from those for its constituent SWNTs within 3% error. Radial deformations of a SWNT were achieved by considering a DWNT with the SWNT as one of its walls and moving radially through the same distance all atoms of the other wall of the DWNT thereby causing a pseudo-pressure through changes in the cumulative van der Waals forces which deform the desired wall. Results of radial expansion/contraction of a SWNT were used to deduce an expression for the van der Waals forces, and find through-the-thickness elastic moduli

(Young's modulus in the radial direction, E_r , and Poisson's ratio $\nu_{r\theta}$) of the SWNT. We have found four out of the five elastic constants of a SWNT taken to be transversely isotropic about a radial line.

MWNTs were studied using the same testing procedures as those used SWNTs. Based on the results from those simulations a continuum model is proposed for a MWNT whose response to mechanical deformations is the same as that of the MWNT. The continuum structure is comprised of concentric cylindrical tubes interconnected by truss elements. Young's modulus, Poisson's ratio, the thickness of each concentric tube, and the stiffness of the truss elements are given. The proposed continuum model is validated by studying its bending and buckling deformations and comparing these results to those from MM simulations.

The major contributions to the field on nanotubes and the scientific literature is a simple and robust continuum model for nanotubes. This model can be used to study both SWNTs and MWNTs in either global or local responses by applying different analytic techniques. This model was developed using a consistent engineering methodology that mimicked traditional engineering testing, assumptions and constraints.

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