6 Conclusions

In summary, the main result from the present work is a transversely isotropic, cylindrical, continuum model for a carbon nanotube. The axis of transverse isotropy is radial, and therefore material properties in the axial and hoop directions are the same. A single wall nanotube (SWNT) is modeled straightforwardly as a cylindrical tube, while a multi-walled nanotube (MWNT) is modeled as nested concentric tubes. The individual walls interact laterally/radially either in unison (rigid gap) or through a pressure interaction. The rigid gap model results in a Euler beam or column model and works well for global bending or buckling deformations and gives results in agreement with those from MM simulations. The pressure interaction model defines the pressure between walls as a function of the wall separation distance. It requires more advanced analysis techniques to apply. Adequate results, as compared to MM simulations, were found by modeling the interaction using truss elements to connect MWNT wall nodes.

The major new contribution to carbon nanotube mechanics lies in employing an engineering approach. In short, nanotube mechanics, and MM simulations, can be approached as macro-level continuum mechanics by using the same methods, assumptions and testing techniques as close to macro-level tests as possible. This idea bears fruition in the virtual experiment method whereby the discretely modeled/simulated nanotube is subjected to deformations similar to those performed by testing machines at the macro-level. The output (energy & deflection rather than load and deflection) is then used to develop a full material response. As a prime example the development of a SWNT isotropic continuum model was determined by using the relationships between the material constants and geometry to find the material properties and wall thickness. This differs from other methods whereby the properties are scaled up from discrete level mathematics to the continuum level, or assumptions are made by atomistic phenomenon (such as bond lengths) which are not necessarily governed by continuum mechanics principles. A similar approach was taken for the investigation of MWNTs, MWNT wall interactions, and the radial response of the nanotube wall. The following sections detail more specific results of this approach.

6.1 SWNTs and the Individual Wall Model

The virtual experiment method was used to determine the properties of a SWNT by subjecting it to various deformations. The strain energy of a nanotube versus its axial deformations was found to be best fit by a third order polynomial. This results in a nonlinear stress-strain response. However, the error involved in treating the response as linear is infinitesimal for small strains. Assuming a linear response for the MM3 potential, it was found that for the equivalent continuum tube, Young's modulus, E = 2.52 TPa, shear modulus, G = 0.96 TPa, Poisson's ratio, ν = 0.21 and wall thickness, t = 1.34 Å. For the Tersoff-Brenner potential the following values were determined; E = 3.10 TPa, G = 0.96 TPa, ν = 0.26 and t = 0.98. The strain energy of bending deformations of the equivalent tube is found to match well with that computed from the molecular mechanics simulations. Also strain energies of the combined axial and torsional deformations computed from the MM simulations matched well with that of the equivalent continuum tube.

6.2 MWNTs and Wall Interactions

Based on the results of MM simulations of DWNTs and a TWNT under various loads, several questions were answered about the similarities/differences of their responses with those of the constituent SWNTs. Based on these results, using the virtual experiment method we proposed a continuum structure whose response to mechanical deformations is the same as that obtained with MM simulations on the DWNT. The proposed equivalent structure differs from that often used and allows for the consideration of van der Waals forces through appropriate truss elements interconnecting concentric tubes. The proposed model was validated by comparing predictions from it for bending and axial buckling deformations with those derived from the MM simulations.

An advantage of having an equivalent continuum structure is that it can be used to compute effective properties of composites comprised of polymers reinforced with MWNTs. Also, an equivalent continuum structure is inherently used to interpret results of experiments on carbon nanotubes and deduce values of material parameters.

Several detailed results can be stated based on the MM simulations results: (i) walls of a MWNT slide freely over each other in both axial and torsional loading of only one wall; (ii) except for buckling deformations, results for a MWNT may be obtained within 3% accuracy from those for the constituent SWNTs subjected to the same traction or displacement boundary conditions; (iii) the wall separation distance is of primary importance when finding energetically favorable MWNT configurations while differences in their helical angles play a minor role in the relative axial translation of walls; (iv) for bending deformations, the choice of a continuum model was found not to be highly important as long as an accurate axial stiffness is used and the radius to wall thickness ratio is high.

6.3 MWNT Buckling and Correlation with SWNTs

The buckling of axially compressed MWNTs was studied by using molecular mechanics simulations, the Euler buckling theory, and the finite element method. The latter two approaches employ continuum structures equivalent to the nanotubes. It was found that the van der Waals forces among atoms on adjacent walls of a MWNT play a significant role. The van der Waals forces cause the MWNT to generally buckle as a unit, that is, the buckled shape is the same for all walls. The present work makes the following new contributions.

For columnar buckling modes, the axial strain at the onset of buckling equaled that given by the Euler column theory. The buckling mode transitions from columnar to shell wall buckling as the tube length is decreased. During the transition columnar buckling modes include crimping which is a form of shell wall buckling. The axial strain at the initiation of the shell wall buckling mode equals the largest of those of the single-walled nanotubes constituting a multi-walled nanotube. An interesting rippling pattern was found in the buckling response of a triple-walled nanotube which illustrates the resistance provided by the individual walls against buckling.

The buckling modes computed from the finite element analysis of equivalent continuum structures, with the van der Waals forces simulated by truss elements, were close to those obtained from the molecular mechanics simulations; however, the transition zone mode shapes were not replicated. Finite element results suggest that

while the consideration of the van der Waals forces is critical, their exact modeling is not very critical as adequate results were found for two different mathematical representations. The modeling of van der Waals forces by truss elements is new and provides an easy way to simulate them. It helps understand how these forces coordinate the buckling of different walls of a nanotube. The magnitude of the van der Waals force can be best computed from equations supplied in the Appendix.

6.4 Radial Wall Properties

A novel MM simulation technique was developed to study uniform radial expansion/contraction of a SWNT. Using these results and the assumption that the equivalent continuum tube is a transversely isotropic material with the axes of transverse isotropy along the radius, the Young's modulus and Poisson's ratio in the radial direction may be determined. For wall thickness of 1.34 Å, the value for which the in-plane isotropic constraints are satisfied, the values of material moduli are $E_z = E_\theta = 2.52$ TPa, $\nu_{\theta z} = \nu_{z\theta} = 0.19$, $E_r = 0.576$ TPa, and $\nu_{r\theta} = 0.0058$. Our value of Young's modulus in the radial direction is nearly one-fourth of that in the axial direction as opposed to Reich et al.'s of one-half. Values of material moduli depend upon the presumed thickness of the wall of SWNT, and the MM potentials used. To our knowledge, there is no experimental data available for Young's modulus of a CNT in the radial direction with which to compare the computed values.