An atomistic-continuum elastic rod model of carbon nanotubes

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The present work focuses on an atomistic-continuum model of single-walled carbon nanotubes (SWNTs) based on an elastic rod theory [1] which can exhibit geometric as well as material nonlinearity. In particular, the SWNT is modeled as a one-dimensional elastic continuum which has some finite thickness bounded by the lateral surface. Exploitation of certain symmetries in the underlying atomic structure leads to suitable representations of the continuum elastic energy [1]. The bridging between the atomic scale and the effective continuum is carried out by parameterization of the continuum elastic energy and determination of the parameters using atomistic simulations.

Elastic properties such as Young's and shear moduli are linearized, isotropic measures that describe material behavior in small strains. However, in SWNTs undergoing large strains, there are effects such as the coupling between extension and twist [2-4] which are not captured by linearized, isotropic moduli. While this is an evidence of anisotropy in large strains, it is of interest to also characterize other deformation couplings in SWNTs. Specifically, the present approach takes into account: (a) bending (b) twist (c) shear (d) extension (e) coupled extension and twist, and (f) coupled bending and shears. Published work on elastic moduli has taken into account (a)-(d) individually for small strains, and past work (including [2-4]) has considered (e). But this is the first effort at a unified large strain approach that takes into account all of these modes for SWNTs.

Further, a two-dimensional membrane model of SWNTs is useful to predict localized effects such as wrinkling or buckling of the effective continuum but may not be computationally efficient to model global behavior of long tubes (microns in length) of interest in nano-oscillators (see, for e.g. [5-6]). A one-dimensional model is better suited to such an application. However, one-dimensional models published so far are limited to linear stress-strain relationships with isotropic material assumptions which do not take into account the aforementioned couplings.

Finally, since this is a parameterized continuum model of an atomic system, it is possible to apply this model, by suitable parameter estimation, to other atomic systems such as silicon or boron nitride nanotubes.

References

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