An atomistic-continuum Cosserat rod model of carbon nanotubes

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The focus of the present work is an atomistic-continuum model of carbon nanotubes (CNTs) based on a Cosserat rod theory [1] which is geometrically and materially nonlinear. In particular, the nanotube is modeled as a 1-dimensional 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. 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 calculated for CNTs in the past like Young's and shear moduli are linearized, isotropic properties applicable to small strain models and may lose validity under large strains. For example, [2-4] deal with the coupling between extension and twist in nanotubes undergoing large deformations using a quasicontinuum 2-dimensional, anisotropic thin-shell model. A model that assumes isotropy of the continuum will be unable to capture this coupling. While this is an evidence of anisotropy in large strains, it is of interest to also characterize the other deformation couplings in a nanotube. Specifically, the present model offers a unified approach to take 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 nanotubes.

Further, most continuum representations of CNTs have been 2-dimensional shell models which are useful for predicting localized effects such as wrinkling or buckling of the continuum but may not be computationally efficient to model global behavior of long tubes (see, for e.g. [5-6]), for which a 1-dimensional model would be better suited. However, the 1-dimensional models published so far have been 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 similar atomic systems as well – e.g., silicon or boron nitride nanotubes.

References

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