

An atomistic-continuum Cosserat rod model of carbon nanotubes

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The focus of the present work [1] is an atomistic-continuum model of single-walled carbon nanotubes (CNTs) based on an elastic rod theory which can exhibit geometric as well as material nonlinearity [2]. In particular, the single-walled carbon nanotube (SWNT) is modeled as a one-dimensional elastic continuum with 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 strain energy density in terms of strain measures that capture extension, twist, bending, and shear deformations [2]. 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 unit-cell atomistic simulations over a range of deformation magnitudes and types. Specifically, the proposed model takes into account (a) bending, (b) twist, (c) shear, (d) extension, (e) coupled extension and twist, and (f) coupled bending and shear deformations. The extracted parameters reveal benefits of accounting for important anisotropic and large-strain effects as improvements over employing traditional, linearly elastic, isotropic, small-strain, continuum models to simulate deformations of atomic systems such as SWNTs. It is envisioned that the proposed approach and the extracted model parameters can serve as a useful input to simulations of SWNT deformations using existing nonlinearly elastic continuum codes based, for example, on the finite element method (FEM).

References

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- [2] Healey T.J., 2002, “Material symmetry and chirality in nonlinearly elastic rods”, *Mathematics and Mechanics of Solids*, **7**, pp. 405-420.

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