ATOMISTIC-CONTINUUM MECHANICAL MODELING OF SINGLE-WALLED CARBON NANOTUBES (SWNTs)

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The present work deals with modeling the mechanical deformation of SWNTs. An atomistic-continuum approach is adopted which incorporates atomistic detail into a continuum analysis. The SWNT is modeled as a two-dimensional hyperelastic membrane in which the continuum strain energy density function is appropriately defined in terms of C-C bond energies over a representative unit cell of the atomic lattice. The bond length deformations are governed by the Cauchy-Born (CB) deformation rule which homogenizes the continuum deformation at the atomic scale. This effectively connects the atomic system to the deformation of the continuum without other phenomenological input, thereby leading to a multi-length scale framework. Essential ideas can be found in other works dealing with deformation analysis of SWNTs [1]. In the case of curved membranes, the CB rule has been modified using the idea of an exponential map [2]. This modification has been adopted in the present work as well. Further, aspects of the CB rule related to spatial inhomogeneity of the deformation at the atomic scale are investigated in the context of a simple class of generalized extension-twist problems [3] in which the kinematic coupling between extension and twist for different SWNTs has also been studied [4]. Stress-strain curves are obtained for SWNTs subject to extension and twist, which serve to estimate the elastic moduli. These values are further validated by computing the components of the elasticity tensor at the onset of deformation. Efforts are currently underway to employ this modeling approach to study the deformation of SWNTs under more complex loading conditions in the context of a finite-element analysis, and preliminary results will be presented.

References

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