

CONTINUUM MECHANICS MODELLING AND FINITE ELEMENT SIMULATIONS OF THE NONLINEAR MECHANICS OF CARBON NANOTUBES

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Molecular theories of elasticity at finite strains are well developed for space-filling crystals [1,2]. The combination of these theories with finite elements gives rise to multi-scale simulations methods capable of handling much larger systems than conventional atomistic calculations [3]. Carbon nanotubes can be seen as graphene sheets rolled into cylinders. They possess a remarkable resilience to mechanical deformation, and display very large elastic deformations. For these reasons, it is tempting to employ the above mentioned techniques for their mechanical analysis. Unfortunately, the standard methods of finite crystal elasticity cannot be applied to crystalline monolayers, particularly with regards to the effect of curvature. A recently proposed generalization of the Cauchy-Born rule, cornerstone of crystal elasticity, which exploits the differential geometry concept of the exponential map, allows to formulate a continuum hyperelastic potential for a surface without thickness replacing the curved graphene sheet [4]. This constitutive model is written explicitly in terms of the atomistic description of the system (here, Brenner's potential), and does not require local atomistic calculations. A continuum version of the non-bonded interactions is also formulated.

Detailed numerical studies involving buckling of nanotubes under different loading conditions demonstrate that the continuum model, discretized with finite elements, very accurately mimics the parent atomistic model in the full nonlinear regime. Our simulations suggest that, in the absence of bond rearrangement or defects, the nonlinear mechanics of carbon nanotubes can be accurately modelled within the strict framework of continuum mechanics, i.e. without any sort of coupled or underlying atomistic calculation. Numerical examples also illustrate the dramatic computational saving which can be achieved for large multi-walled nanotubes, and replicate some unusual features observed in experiments. The application of the continuum model to the design of nanodevices is also illustrated.

References

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