Atomistic-continuum mechanical modeling of single-walled carbon nanotubes

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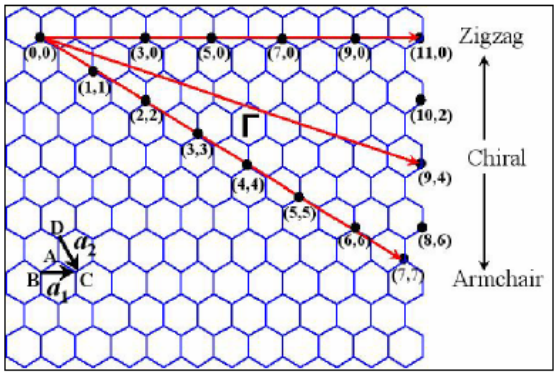
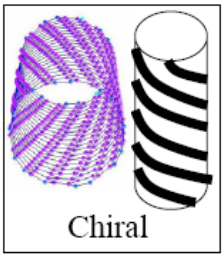
Carbon nanotubes possess remarkable electrical, thermal and mechanical properties, and their potential applications include such diverse areas as conductive and high strength composites, energy storage and conversion devices, sensors, field emission displays and radiation sources, hydrogen storage media, and nanometer sized semiconductor devices, probes and interconnects. Although much progress has been made in performing nanoscale experiments, it is necessary to develop modeling and simulation tools to further these findings and provide insight into experimental results. This talk reports on our ongoing work in modeling mechanical deformations of single-walled carbon nanotubes (SWNTs) using enriched continuum models which incorporate atomistic detail into a continuum analysis.



Planar Graphene Sheet



The talk focuses on two continuum models of SWNTs – a two-dimensional elastic membrane model, and a one-dimensional rod model – in which the continuum strain energies are determined from analytic interatomic potentials and atomistic simulations. The two-dimensional membrane model has been employed in the past for predicting localized effects such as wrinkling or buckling of the effective continuum. The one-dimensional rod model for SWNTs is a recent effort for modeling the global behavior of long SWNTs and is more computationally efficient. Numerical results on the elastic moduli for different deformation modes of SWNTs like extension, twist, bending and shear using these models, will be presented. It will also be demonstrated that certain phenomena like extension-twist coupling and bending-shear coupling that standard, isotropic, linear elastic models are unable to quantify, can be captured by such atomistic-continuum models in a unified manner.