Nanomechanics of graphene nanoscrolls

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The rapid development of synthesis and characterization of nanostructured materials as well as unprecedented computational power have brought forth a new era of materials research in which experiments, simulation and modeling are performed side by side to probe the unique mechanical properties of nanoscale materials. This talk aims to present an overview of our recent studies of the mechanical properties of carbon nanoscroll-based nanomaterials and nanodevices via molecular dynamics simulations and continuum mechanics modeling. Molecular dynamics simulations and theoretical analyses are performed to probe equilibrium and dynamic properties of carbon nanoscrolls -- made of a continuous basal graphene sheet rolled up in a spiral form -- such as their equilibrium core size as well as their oscillatory and translational motion with and without an external controlling field. By analyzing the elastic bending and surface interaction energies in the system, we have developed equations of motion in terms of the surface energy, the bending stiffness, the interlayer spacing, the length and width of the basal graphene sheet and the core radius of the nanoscroll. The results suggest that the carbon nanoscrolls hold great promises for applications such as nano-oscillators, nanoactuators, nanomotors, tunable water and ion channels, nanofluidic devices, nanofilters as well as tunable gene and drug delivery systems [1-6].

References