Bending of Nanotubes, Nanoscale Beams and Sheets

Faculty Collaborators

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Overview of Current Investigations

The goal of this project it to develop accurate material models of multi-walled carbon nanotubes and to use these models to analyze the response of nanotubes to applied bending loads. An important related question is how bending changes the electrical and chemical properties of nanotubes. Experimental work reveals that, during bending, multi-walled carbon nanotubes develop wrinkles on their compressed side. These wrinkles appear to strongly affect the properties of bent tubes. In particular, it has been discovered that kinks and wrinkles on the surface of carbon nanotubes exhibit enhanced chemical activity. Since the bending of carbon nanotubes is completely reversible for deformations leading to wrinkling, so called ``kinky" chemistry studies have been conducted to selectively modify the carbon nanotubes at the wrinkled zones.

We are examining the bending of multi-walled nanotubes within the framework of nonlinear continuum mechanics. By using the Principle of Virtual Work (PVW) and appropriate constitutive assumptions, we obtain equilibrium equations for the in-plane bending of nonlinear elastic shells. Following earlier work on the bending of thin-walled pipes, we treat wrinkling in nanotubes as a bifurcation in the solutions to the governing equilibrium equations. The novel feature of our equations for bending is the inclusion of van der Waals forces acting between adjacent walls in a multi-walled nanotube; the treatment of the terms that arise from the inclusion of these interaction forces cannot be subsumed under standard mathematical techniques.

We combine continuum modeling with Molecular Dynamics (MD) and Quantum Mechanics (QM) computational simulations. Simulations of the bending of small-diameter single- and multi-walled nanotubes yield information on both the bulk properties of nanotubes and on how these bulk properties change during bending. This information can then be incorporated, via constitutive theory, into the continuum modeling of bending. To examine the bending of larger-diameter multi-walled nanotubes, information on the global geometry of bent tubes derived from continuum modeling can be passed as boundary conditions to QM/MD simulations, which can then be used to study the mechanical behavior and the chemical properties of the multi-walled nanotubes just near the high-curvature, wrinkled regions.

For example, using a combination of continuum modeling, atomistic simulations, and numerical optimization, we estimate the bending stiffness of a graphene sheet. We consider a rectangular sheet that is initially parallel to a rigid substrate. The sheet interacts with the substrate by van der Waals forces and deflects in response to loading on a pair of opposite edges. To estimate the bending stiffness, we model the graphene sheet as a continuum and numerically solve an appropriate differential equation for the transverse deflection. This solution depends on the bending stiffness. We then use an optimization procedure to find the value of the bending stiffness that minimizes the difference between the numerical solutions and the deflections predicted by atomistic simulations.

Publications

1. "Measuring and Modeling Thermal Fluctuations at Nanometer Length Scales", R. M. Ralich, R. D. Ramsier, D. D. Quinn, C. B. Clemons, and G. W. Young, *Phys. Rev E*, Vol. 65 (2002), pp. 057601-1-4.

2. "Buckling Instabilities in Coupled Nanobeams", D. D. Quinn, A. E. Pudloski, C. B. Clemons, J. P. Wilber, G. W. Young, and A. Buldum, *ENOC-2005*, Eindhoven, Netherlands, August (2005), pp. 1-8.

3. "Buckling Instabilities in Coupled Nanoscale Structures", A. E. Pudloski, C. B. Clemons, J. P. Wilber, G. W. Young, A. Buldum, and D. D. Quinn, *2005 ASME International Mechanical Engineering Congress and Exposition*, Orlando, Florida, November (2005), pp. 1-9.

4. "Continuum and atomistic modeling of interacting graphene layers", J.P. Wilber, C. B. Clemons, G. W. Young, A. Buldum and D.D Quinn, *Phys. Rev. B*, Vol. 75 (2006), pp. 045418-1 – 045418-10.

5. "Buckling Instabilities in Coupled Nano-Layers", D. D. Quinn, C. B. Clemons, J. P. Wilber, G. W. Young and A. Buldum, *International Journal of Non-Linear Mechanics*, Vol. 42 (2007), pp. 681-689.

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1. NSF Division of Mathematical Sciences - "Modeling, Simulation, and Analysis of Bending Nanotubes" NSF Grant No. DMS-04-07361, (2004 - 2008): $267,935, P. Wilber - PI, D. Quinn, D. Golovaty, G. W. Young and A. Buldum.