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MRSEC SEMINAR SERIES

Multiscale Modeling of Carbon Nanosystems: Bulk Dynamic Response and Phonon Dispersion

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Date: Tuesday, August 27, 2013

Time: 3:00 PM

Location: Klaus, Room 1116W

Abstract:
This talk will detail multiscale computational models for predicting bulk dynamic response and phonon spectra/dispersion in carbon nanostructures. The first half of the talk will discuss multiscale modeling of curved and twisted carbon nanotubes (CNT's) using an atomistically-informed continuum theory governing the dynamics of curved and twisted, anisotropic beams. The theory represents the system using intrinsic curvature and strain, which allows low-order interpolation functions to describe generally curved and twisted nanotube center-lines. The computational model is able to capture the nanotube's bulk dynamic response, without the expense of calculating the dynamic response of individual atoms. Results from the simulations are compared to similar CNT results available in the literature, and close agreement is noted. The second half of the talk will discuss multiscale continuum-atomistic models for predicting phonon dispersion in carbon nanostructures, to include graphene sheets and CNTs. The prediction of phonon dispersion is typically accomplished using either semiclassical techniques, such as lattice dynamics, or quantum mechanical techniques based on second quantization and creation/annihilation operators. In both cases, the calculations can be tedious and require accounting for three degrees of freedom for every atom in the unit cell. For carbon nanostructures, even pristine unit cells can be large – e.g., a relatively small diameter carbon nanotube (CNT) has 1708 atoms in its unit cell. If defects are to be studied, a supercell approach can easily exceed 10,000 degrees of freedom or more. To overcome these issues, reusable shell-like finite elements are developed and incorporated into a Bloch analysis procedure for computing the dispersion relationships. Due to the use of an underlying continuum formulation, the dispersion curves are accurate at relatively low frequencies and long wavelengths. This is not overly restrictive, however, since these branches (and in particular the acoustic variants) are of primary interest in many instances, such as in predicting thermal properties where only acoustic branches are typically considered due to their predominance in terms of excited numbers, and their much higher group velocities. The validity of the technique, and the frequency and wavenumber range for which it is applicable, are detailed via comparisons of computed results to those found in the literature.