PHONON GREEN'S FUNCTION FOR CALCULATION OF FREQUENCIES IN NANOTUBES CONTAINING DEFECTS

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Practical application of single-wall carbon nanotubes in electronics and other devices requires their precise characterization in terms of chirality and other characteristics such as internal strains, discrete atomistic arrangements in the lattice, and presence of lattice defects. Measurement of phonon frequencies through optical spectroscopy has been found to be a very useful tool for characterizing single-wall carbon nanotubes. Calculations of phonon spectra of perfect single-wall carbon nanotubes are available in the literature, but the effect of lattice defects on phonons has not yet been calculated. A real nanotube almost always has lattice defects such as extra atoms attached to a carbon atom, missing or additional atoms, branching etc. I will describe a fully atomistic model for calculating the phonon dispersion relations of a single-wall carbon nanotube containing a point defect. The model is useful for interpretation of optical spectra and extracting useful information for characterizing the nanotubes. The phonons will be represented in terms of causal Green's function that will be calculated by using the Born-von Karman type model and the force constants derived from a recently calculated interatomic potential between carbon atoms in a nanotube. This model includes off-diagonal force constants in contrast to some previous models in which force constant matrices were assumed to be diagonal. The effect of the defect is represented by a change in the phonon Hamiltonian. The corresponding defect Green's function is calculated by solving the Dyson equation in the defect space. The phonon frequencies are calculated from the poles of the defect Green's function whereas the phonon density of states is obtained from the imaginary part of the defect Green's function. Raman and infrared active modes are separately identified. Numerical results will be presented for lattice defects in single-wall carbon nanotubes with different chiralities.

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