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Vibrational Behavior of Single-Walled Carbon Nanotubes: Atomistic Simulations

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This study examines the vibrational behaviors of both armchair and zigzag carbon nanotubes (CNTs). The natural longitudinal/flexural/torsional/radial frequencies of CNTs were extracted and analyzed simultaneously from an equilibrium molecular dynamics simulation without imposing any initial modal displacement or force. Initial random atomic velocities, which were assigned to fit the simulated temperature, could be considered as an excitation on CNTs composing of wide range of spatial frequencies. The position and velocity of each atom at every time step was calculated using finite difference algorithm, and fast Fourier transform was used to perform time-to-frequency domain transform. The effects of CNT length, radius, chirality, and boundary condition on the vibrational behaviors of CNTs were systematically examined. Moreover, the simulated natural frequencies and mode shapes were compared with the predictions based on continuum theories, i.e., rod, Euler-Bernoulli beam and nonlocal Timoshenko beam, to examine their applicability in nanostructures.

Keywords: Natural frequency, Mode shape, Molecular dynamics, Carbon nanotube, Radial breathing