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Energy dissipation and phononic friction in carbon nanotube oscillators

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ABSTRACT

In this work, we compute the phonon properties of carbon nanotube using finite difference method and DFPT approach separately for comparison. We found that both methods produce very similar phonon frequencies near the G-point. However, in the high frequency range, the optical phonons from both methods differ significantly. We attribute this difference to the variation of accuracies in atomic force computation in both methods.

Keywords: Carbon nanotube, phonon, oscillator, friction

1. INTRODUCTION

Recently there has been a rapid progress in design and fabrication of devices at atomic scale. The report of linear mechanical oscillations in multiwalled carbon nanotubes (CNTs) with ultra low friction[1] presented a feasible system to understand fundamental physics of nanoscale motions. The process of extruding out the inner CNT causes excess vdW energy to the system. And this excess vdW energy pushes the inner core towards the minimum potential energy position (to the middle of the oscillator). This push gives kinetic energy to the inner core with which it moves past the middle position and reaches the other end of CNT and thus commences oscillations. Frequency of these oscillations can be up to several gigahertz[2]. Although there have been numerous studies on CNT linear oscillators[2-4], a lack of understanding on detailed mechanism of friction (where kinetic energy at sliding interfaces will be converted into lattice vibrations or phonons) hinders progress on finding ways to control the damping.

Due to the incommesurate nature of the interface, the lateral forces between sliding atomic surfaces are organized such that the average sliding force is minimized. This superlubricity has been experimentally observed in several systems[1, 5]. However, various other energy dissipation channels due to nonequilibrium phonons persist and cause damping of the oscillatory motion. In this work, we compute the phonon properties of (10,10) CNT using finite difference method and DFPT approach separately for comparison. The computed phonon properties from

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finite difference method are used to generate phonon wavepackets and the propagation of such phonon wavepacket of certain frequency and polarization on the outer CNT of oscillator is studied using molecular dynamics simulations.

2. METHODOLOGY

DFT calculates phonon properties of pure materials and closely matches with experimental results[6]. Phonon vibrational properties of outer CNT of the oscillator, which is a pristine (10,10) SWCNT are computed from first-principles using density functional perturbation theory (DFPT)[7] at the GGA-PBE level. An alternative approach would be force field based finite displacement method which requires relatively large supercell. DFPT not only avoids the problem of large supercells, it includes long-range polarization fields due to optical phonons. The ground state results of primitive unit cells can be processed to displace atoms arbitrarily (and infinitesimally) and the responses are computed by means of perturbation theory. For phonon calculations, 1 X 1 X 2 super cell was used, which comprises of 80 C atoms. Calculation up to the G-point have been performed by using Vienna *ab initio* simulation program (VASP). The cutoff energy of plane-wave basis is 500 eV, and the convergence criteria of 1E-8 eV/A is used for ionic relaxation as well as lattice vibrational calculations. Then using G-point results, we computed the phonon dispersion relation and phonon eigen vectors of pristine (10,10) CNT unitcell via PHONOPY software[8].

Phonon properties are also obtained using finite-displacement method or supercell method[9] which constructs the force-constant matrix through the resultant forces of all atoms in supercell by displacing the ions individually (small enough displacement to maintain harmonicity) in unitcell. (10,10) CNT of 1000 unitcells is minimized at ground state. Small displacement (0.01 A) is imposed separately on each atom of one unitcell and resultant forces on all atoms of 1000 unitcells are computed. Force-constant matrix is constructed using these forces. Fourier transform of this force-constant matrix is the dynamical matrix, diagonalsing which resulted in phonon frequencies and phonon modes at particular wave vector. Relation between frequencies and wave vector gives the dispersion relation.

3. RESULTS AND DISCUSSION

Near G-point, both methods are found to generate very similar phonon frequency values. However, as the wave vector increases, results of both methods diverge significantly. At high frequency range, the optical phonons from both methods differ by almost 40 meV which is a significant difference. We attribute this variation in optical phonon frequencies to an ensemble of

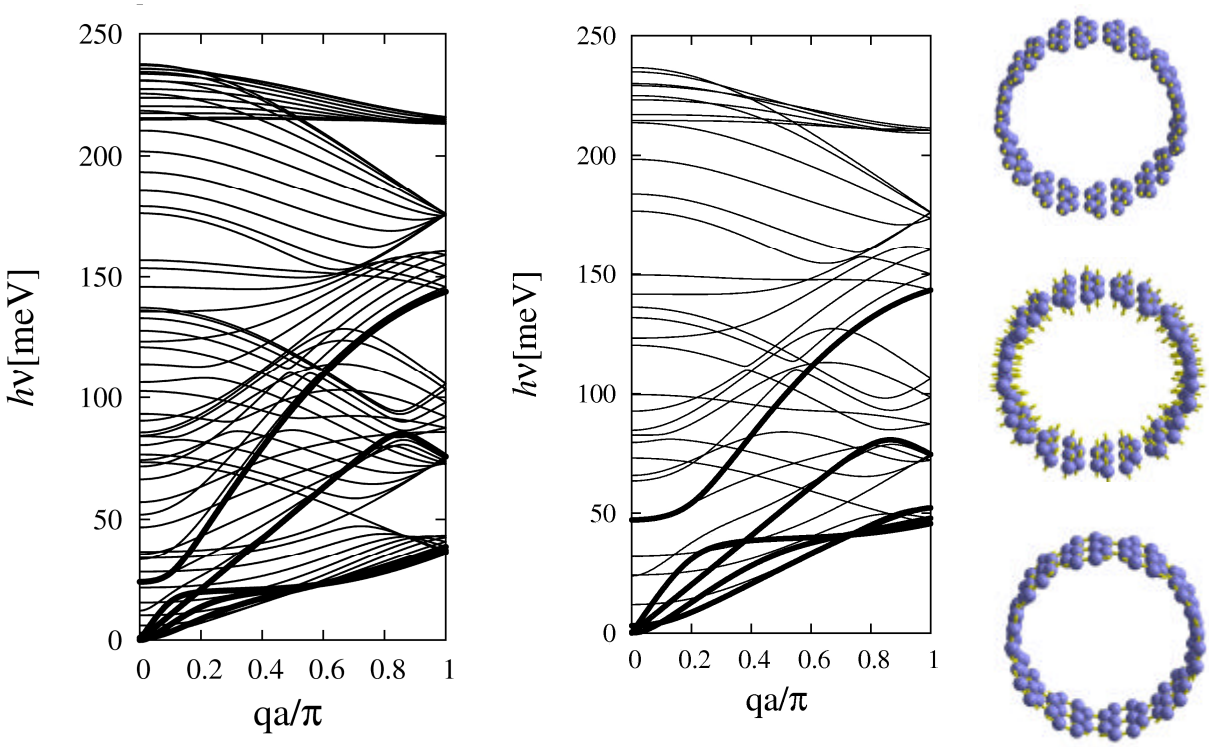

Figure 1. Phonon dispersion (left panel: (10,10) CNT, middle panel: (5,5)) and symmetry of phonon modes (in right panel, LA, BR and TW modes from top to bottom) of a (10,10) CNT. *v* is frequency, 'a' is unitcell size, and *h* is Planck constant.

reasons viz. relatively inefficient force field models compared to *ab initio* force values, DFPT results are free of anharmonic contributions.

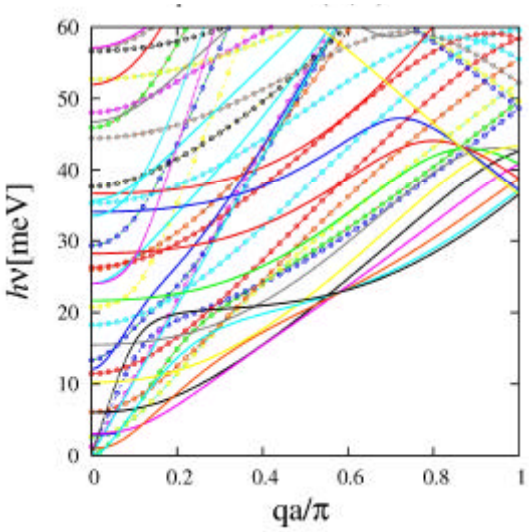

Figure 2. Comparison of dispersion relations of (10,10) CNT computed by finite difference method (lines) and DFPT(points)

4. CONCLUSIONS

In summary, we presented the computational procedure to generate the phonon dispersion for carbon nanotubes using finite difference method and DFPT approach. The computed phonon properties from finite difference method will be used to generate phonon wavepackets. Propagation of such phonon wavepacket of certain frequency and polarization on the outer CNT of oscillator is studied using molecular dynamics simulations.

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