# Mechanical wave propagation in carbon nanotubes driven by an oscillating tip actuator

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We investigate the mechanical wave propagation in single-walled carbon nanotubes (SWNTs) induced by two oscillating tips, using molecular dynamics simulations. We found a mandatory correlation condition between the tip oscillation frequency and magnitude in order to generate a quasi-steady-state standing wave with a characteristic wavelength and frequency changing with the tube radius, but independent of tip conditions. Our findings suggest the possibility of using SWNTs as nanopumping systems for potential applications of fluid transport and drug delivery. © *2009 American Institute of Physics*. [DOI: 10.1063/1.3068312]

Since their discovery, carbon nanotubes (CNTs) attracted a lot of interest due to their many interesting structural, mechanical, and electronic properties and a wide range of potential applications. Many applications of CNTs are closely related to their mechanical properties, in particular, mechanical wave propagation in CNTs, such as nanoactuators,[1] mechanoelectronic devices,[2,3] pressure sensors,[3–7] and drug delivery devices.[8–10] Therefore, the study of wave propagation in CNTs is of both scientific and technological significance.

In recent years, a number of studies of wave propagation in CNTs have been carried out through theoretical modeling and computer simulation.[11–18] Li and Chou[12] studied elastic wave propagation in single-walled nanotubes (SWNTs) by atomistic simulation using the structural mechanics method. The wavelength and velocities of longitudinal, transverse, and torsional waves were obtained, and a relationship between the wavelength and wave frequency was established. Wang and Hu[13] carried out a detailed study of the flexural wave dispersion in SWNTs using molecular dynamics (MD) simulations. They found that the traditional Timoshenko beam theory is able to provide a good description for the flexural wave dispersion with small wave numbers, while the microstructure of the CNTs plays an important role in the flexural wave dispersion with large wave numbers. A theoretical approach was proposed by Natsuki *et al.*[14] to calculate the elastic wave propagation in CNTs. It was shown that the wave velocity in SWNTs changes with the increasing wave frequency. Wang[15] analyzed CNT wave characteristics by applying nonlocal Euler–Bernoulli and Timoshenko beam models. Wavelength and its diameter dependence were explicitly derived from nonlocal continuum models.

So far, only intrinsic properties of wave propagation in CNTs have been studied without considering the effects of the external stimuli that generate the waves in CNTs. The main objective of the present study is to extend the previous studies by including the effects of external stimuli. We will simulate the mechanical waves being generated by local deformation in SWNTs, specifically by two oscillating tips, and investigate the resulting wave propagation properties using MD simulations. We study not only the intrinsic effects, such as tube diameter and tube length, but also the extrinsic effects, such as tip pressing frequency and local deformation magnitude on the characteristic wavelengths and wave velocities of the propagating waves in SWNTs.

We used the same MD method and algorithm as used before[5–7] for studying SWNTs under hydrostatic pressure. Since SWNTs are known to have isotropic mechanical properties,[7] only zigzag SWNTs of different diameters ranging from (8,0), (10,0), (13,0), (15,0), to (17,0) were used. The simulation setup and procedure is shown in Fig. 1. We use a SWNT of finite length with two free open ends. The local deformation is applied by two hard-wall tips pressing the tube from top to bottom, as shown in Fig. 1. The $Y$-coordinates of all the carbon atoms fall in between the tips in the $XZ$ plane are pressed downward and upward by a

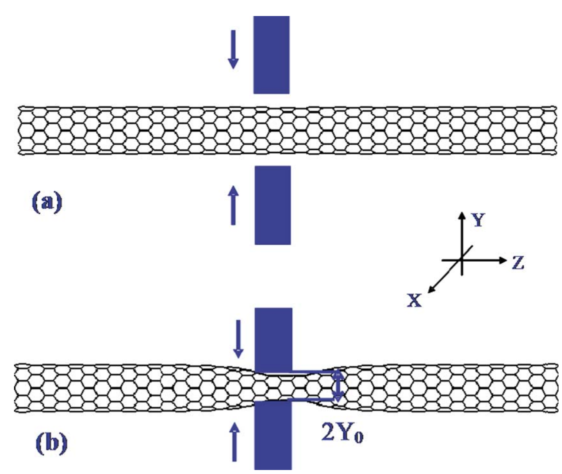


FIG. 1. (Color online) Schematic of radial deformation in a SWNT induced by pressing two tips. (a) Before tip pressing. (b) After tip pressing. The final distance between the tips is $2Y_0$.

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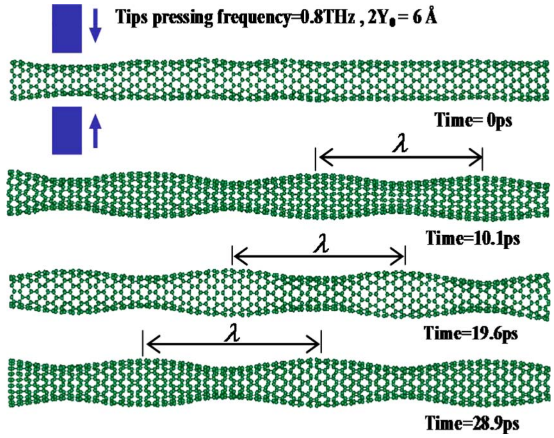


FIG. 2. (Color online) Standing mechanical waves generated by two tips oscillating continuously at a fixed frequency at the left end of a (10,0) SWNT. The tip pressing frequency is 0.8 THz. The magnitude of tip motion is $2Y_0=6$ Å. The tube length is 136 Å.

hard-wall interaction with the tips to the maximum deformation magnitude (final tube thickness in the $YZ$ plane) of $2Y_0$ as indicated in Fig. 1(b). As the tips move and oscillate, MD simulations were carried out at 300 K to investigate the mechanical response of SWNT to the tip motion.

If the tips are pressed only once and fixed at the final distance of $2Y_0$, a mechanical wave is observed to be generated propagating away from the tip position. As the wave travels along the tube, it dissipates the mechanical energy (deformation energy) input by the tips. Consequently, the wave gradually dies out. Typically, we found that the wave disappears after about 10 ps. In order to keep a sustained traveling wave in the SWNTs, we then oscillate the tips by pressing and releasing at a chosen frequency to continuously pump the energy into the systems. In this way, standing mechanical waves are successfully generated in the SWNTs.

Figure 2 shows an example of simulation. The tips are placed at the left end of the nanotube. As the wave is generated, it propagates along the nanotube to the right until it reaches the right end of the nanotube, then a reflection wave is created, which propagates back to the left along the nanotube. As discussed by Li and Chou,[12] the reflected waves traveling backward may initially interfere with the original waves traveling forward, both propagating back and forth in the nanotube. Eventually, the system reaches a quasisteady state forming a standing wave with a fixed wave wavelength and wave velocity, as shown in Fig. 2. The wavelength ($\lambda$) of the standing wave has been measured from the snapshots of simulations (see Fig. 2) and statistically averaged over different wave periods in one nanotube and over time. The time period ($T$) of the standing wave has also been measured by recording the time interval within which one point in the nanotube reaches its crest twice during the propagation of the standing wave. Then, the wave frequency is simply $f=1/T$ and the wave velocity is calculated as $v=\lambda f$.

One focus of our study is to investigate how mechanical wave can be generated by external forces, e.g., by using an actuator consisting of two oscillating tips as illustrated in Fig. 1. We will first examine the dependence of mechanical wave on extrinsic effects of tip conditions, i.e., the tip oscillation frequency and magnitude. Most importantly, we found that not all tip conditions can lead to the steady-state wave propagation. There exists a mandatory correlation between the tip oscillation frequency and tip oscillation magnitude in order to drive the mechanical wave in the nanotube to reach a quasisteady state. The standing wave can only form by matching a given tip oscillation magnitude ($Y_0$) with an optimized tip frequency, as shown for the (10,0) tube in Table I. Such matching relationships are found for all nanotubes simulated. In general, the larger the tip oscillation magnitude (corresponding to the smaller $Y_0$ value), the lower the tip oscillation frequency is required. The exact quantitative matching ratio between the magnitude and frequency varies with nanotube radius.

Another important point we found is that as long as a good match between the tip oscillation magnitude and frequency is found, the steady-state standing wave generated in the (10,0) SWNT has the same frequency (~1.67 THz), wavelength (~43.64 Å), and velocity (~7.28 km/s), independent of the actual tip magnitude and frequency used as shown in Table I. This indicates that the steady-state solution of standing wave frequency, wavelength, and velocity are unique characteristics of the (10,0) SWNT determined by the intrinsic properties of the tube, in particular tube radius (see discussion below). The extrinsic tip effects cannot change the intrinsic tube properties. On the other hand, the extrinsic tip effects must be chosen to resonate in a way so that the characteristic steady-state solution can be reached and sustained. Especially, the tip oscillations need to input approximately the same amount of power (i.e., the same mechanical energy per unit time) to drive the mechanical wave in the SWNT.

The simulations also show that at a given tip driving power, the lifetime of the quasi-steady-state mechanical wave is limited for a given nanotube length. The generated standing wave can last longer in a short tube than in a longer tube. The wave dies out sooner in a longer tube because the tip power input cannot keep up with the faster and larger mechanical wave energy dissipation in a longer tube. On the other hand, for a given tube length, it is found that using a higher tip oscillation frequency with a smaller magnitude can

TABLE I. The correlated tip oscillation magnitudes and frequencies used in driving the steady-state standing wave in a (10,0) CNT.

| Tip magnitude $2Y_0$ (Å) | Tip frequency (THz) | Wave frequency (THz) | Wave wavelength (Å) | Wave velocity (km/s) |
|---|---|---|---|---|
| 4.0 | 0.416 | $1.65 \pm 0.07$ | $43.81 \pm 1.11$ | $7.23 \pm 0.48$ |
| 5.0 | 0.556 | $1.68 \pm 0.07$ | $43.83 \pm 0.72$ | $7.36 \pm 0.40$ |
| 6.0 | 0.833 | $1.67 \pm 0.10$ | $43.27 \pm 0.75$ | $7.24 \pm 0.40$ |

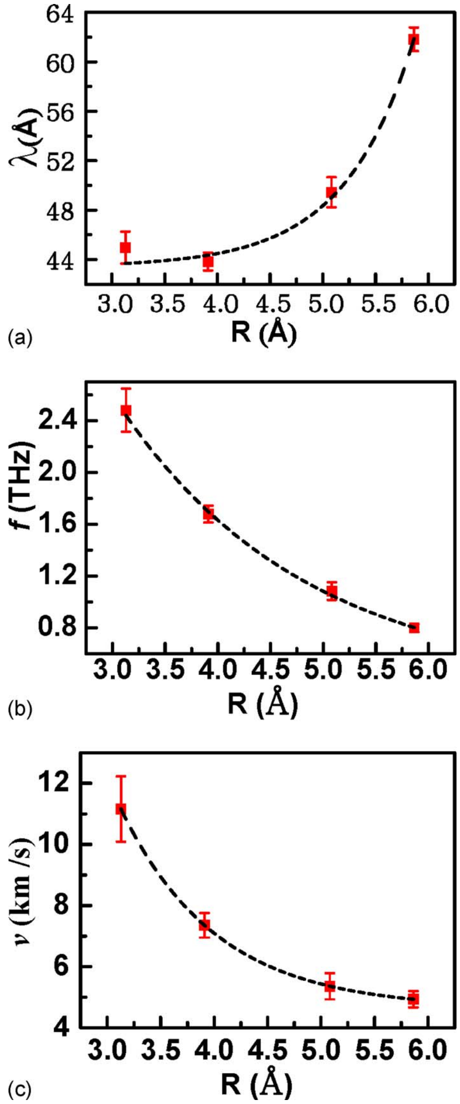


FIG. 3. (Color online) The simulated characteristic wavelength, frequency, and velocity of the steady-state standing wave as a function of tube radius, generated by tip oscillations using $2Y_0=5$ Å. The red squares are simulated data with error bars. The dashed line is an exponential fit to the data.

sustain the steady-state mechanical wave for a longer time. This is possibly because on the one hand, the higher driving tip frequency has a higher "horsepower" injecting more energy per unit time into the tube, and on the other hand, the smaller tip oscillation magnitude produces a smaller wave magnitude, which minimizes the wave energy dissipation rate.

Next, we examine the dependence of characteristic standing wave wavelength, frequency, and velocity on intrinsic tube properties, i.e., the SWNT radius and length. Figure 3 shows the simulated characteristic wavelength ($\lambda$), frequency ($f$), and velocity ($v$) of the steady-state standing wave as a function of tube radius ($R$). For the simulated tube radii ranging from 3.0 to 6.0 Å, the generated mechanical wave has the typical wavelength ranging from ~40 to ~60 Å [Fig. 3(a)], the frequency in the terahertz range [Fig. 3(b)] and the velocity reaching tens of kilometers per second. Our simulations show that the wavelength increases, while frequency and velocity decrease with increasing radius, all "exponentially" as indicated by the perfect exponential fit (dashed lines) to the data (red square dots) shown in Fig. 3. Such dependence can be understood by considering the SWNT as the continuum elastic medium in the shell model. As the tube radius becomes larger, the tube becomes softer (smaller modulus)[5–7,18] so that the wave wavelength increases and frequency decreases, just like in a typical tubular music instrument. The decrease in wave velocity with the increasing radius indicates that frequency decreases faster than the wavelength increases with the increasing radius.

We also carried out simulations for different tube lengths and found that the characteristic wavelength, frequency, and velocity of the partial standing wave are independent of tube length. This seems to indicate that for a given tube radius, only the corresponding characteristic wavelength is sustainable in a quasisteady state, while other wavelengths are unstable and die out quickly. The underlying physical mechanism for this phenomenon needs further study.

In summary, using MD simulations we have demonstrated the possibility of using two oscillating tips (such as AFM tips or cantilever mounted tips) to generate sustained mechanical wave propagation in a SWNT. We found a mandatory correlation condition between the tip oscillation frequency and magnitude for the generated mechanical wave to reach a quasisteady state, whose lifetime can be increased by using higher tip frequencies and smaller tip magnitudes. The lifetime also increases with the decreasing tube length. The characteristic wavelength and frequency of the steady-state standing wave is only determined by the intrinsic tube properties, i.e., the tube radius, independent of the extrinsic tip effects. Our findings may have useful implications in making CNT-based nanomechanical devices, such as nanopumping for fluid transport and drug delivery.

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