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Phonon wave-packet scattering and energy dissipation dynamics in carbon nanotube oscillators

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Friction in carbon nanotube (CNT) oscillators can be explained in terms of the interplay between low frequency mechanical motions and high frequency vibrational modes of the sliding surfaces. We analyze single mode phonon wave packet dynamics of CNT based mechanical oscillators, with cores either stationary or sliding with moderate velocities, and study how various individual phonons travel through the outer CNT, interact with the inner nanostructure, and undergo scattering. Two acoustic modes (longitudinal and transverse) and one optical mode (flexural optical) are found to be responsible for the major portion of friction in these oscillators: the transmission functions display a significant dip in the rather narrow frequency range of 5–15 meV. We also find that the profile of the dip is characteristic of the inner core. In contrast, radial breathing and twisting modes, which are dominant in thermal transport, display ideal transmission at all frequencies. We also observe polarization dependent scattering and find that the scattering dynamics comprises of an oscillating decay of localized energy inside the inner CNT. This work provides a way towards engineering CNT linear oscillators with better tribological properties.

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I. INTRODUCTION

Friction during the relative motion of two atomic surfaces arises from an exchange of energy between the surfaces. For strongly interacting surfaces, friction involves large stress and displacement fields, rearrangement of interatomic bonds, and loss or exchange of atoms at the interface. In case of weakly interacting interfaces, which is the focus of this work, friction amounts to the dissipation of energy through phonon excitations and electronic excitations.

Cumings and Zettl’s experimental work on multiwalled carbon nanotube (MWCNT) pull-out set the stage for CNT based oscillators, actuators, and bearings. While telescoping out the inner walls, they quantified the dynamic (static) friction force between the walls as less than 4.3 × 10⁻¹⁵ N/Å² (less than 6.6 × 10⁻¹⁵ N/Å²), which are almost three orders smaller than friction forces in current MEMS. Around the same time, Kolmogorov and Crespi’s computational work on smooth intershell mobility between the walls of commensurate MWCNTs introduced the possibility of NEMS operating at Gigahertz range. In a recent experimental work, this ultra-smooth sliding under ambient conditions is observed even in a centimeter long DWCNT. And very recently, Ma et al. proposed an analytical model for the critical length above which such superlubricity breaks down. Various nanoscale mechanical devices have been proposed since then that take advantage of the relative motion of carbon nanotube walls, such as: nanobearing, nanoelectromechanical systems, non-volatile memory devices, nanoresonator, nanoresonator, nanosensor, nanomotor, nanogear, nanobolt-nut pair, nanoaccelerometer, nanoresonator, nanomach, high performance FETs, Brownian motor, inertial measurement systems, etc.

During the first half of the previous decade, various studies based on classical molecular dynamics have attempted to address the role of commensuration, boundary conditions, functionalization, defects, interwall distance, length of sliding surfaces/overlap/telescoping, and temperature in energy dissipation in CNT based linear oscillators. There have been conflicting findings in regard to sliding forces in commensurate vs. incommensurate systems. Incommensurate systems were found less dissipative than commensurate systems; however, Tangney et al. claimed that dynamical friction was independent of commensuration of bitubes and of the overlap area between tubes. They further claimed that the source of friction was the motion of tube ends (surface edges), which depended on the relative velocity of tubes. Zhao and Cummings investigated these differences and found the outcome to depend on temperature, commensuration, and type of molecular dynamics ensemble adopted. In an attempt to resolve the conflicting findings on the effect of commensurability, Zhu et al. identified interaction strength and intertube energy corrugation as two crucial parameters in assessing the effect of commensurability on energy dissipation, yet the underlying physics need to be investigated.

Stone-Wales and vacancies have been found to excite low frequency vibrational modes and to markedly increase the dissipation rate. However, a single Stone-Wales
defect was found to suppress dissipation in a linear oscillator by avoiding rotational motion.\textsuperscript{43} Although dissipation rate was typically found to increase linearly with temperature in most studies, Chen \textit{et al.}\textsuperscript{52} reported an inverse relation at ultra-low temperature ranges ($\approx 0.01$ K–1 K): the critical temperature at which the inversion occurred corresponded to the saturation of thermal lubrication and the appearance of phononic friction. The critical temperature in turn was related inversely with the CNT length.

Phononic friction at the interfaces involving adsorbed monolayers has been studied both experimentally and theoretically. The experimental works involved hydrogen and deuterium terminated Si surfaces,\textsuperscript{55} H$_2$O, N, superheated He films adsorbed on Pb(111) substrates,\textsuperscript{56} and adsorbed films of several inert gas atoms and hydrocarbons on various metallic substrates as reported in Ref. 57. The theoretical works involved CO molecule adsorbed on the (100) face of Cu.\textsuperscript{58} Although a few pioneering experimental works,\textsuperscript{8,12,28,59} have addressed friction in sliding nanotubes, these are all phenomenological in nature, and to our knowledge, phononic friction in CNT oscillators has not yet been subjected to theoretical or experimental investigations.

Recent theoretical attempts\textsuperscript{60,61} on thermal energy exchange at the interfaces of CNT confirmed a strong dependence of frequency and polarization of phonons and also of interface characteristics. In the area of interfacial thermal transport, a variety of CNT interface configurations such as surface-surface interface,\textsuperscript{60,62,63} end-end interface\textsuperscript{64} and CNT-substrate interface\textsuperscript{65} have been studied. In order to understand the effect of interface bonding and spacing on thermal transport, most of these studies analyzed individual phonon scattering mechanism at the interfaces. In an MD based study, Greaney and Grossman\textsuperscript{63} observed a resonance based energy transfer between CNTs when positioned side by side. Kumar and Murthy\textsuperscript{60} used heat pulse propagation and wavelet analysis to identify dominant phonon modes in thermal transport across CNTs when CNTs were positioned perpendicular to each other.

In CNT oscillators, deformations such as bending and wavy modes of outer CNT, which are manifested by the collective excitation of disorderly phonon modes, have been identified as the major channels through which the translational kinetic energy of the core dissipates as thermal energy.\textsuperscript{48,50,65} Exchange of vibrational energy from useful mechanical motion to thermal fluctuations and vice-versa have so far not involved any phonon level treatment. Phonon wave packet formalism\textsuperscript{66} provides a powerful computational framework for treating single phonon transport across interfaces.\textsuperscript{54,66,67} Using this scheme, the dynamics of single mode phonon at the sliding CNT interface can be studied.

Once the motion of core initiates, a typical oscillation cycle involves: motion along the outer CNT where a part of orderly translational energy dissipates in to disorderly high frequency phonon modes; reversal of motion of core at the ends of outer CNT. The focus of the present work is on the energy exchange dynamics between orderly translation motion of core and phonon modes of outer CNT. The fundamental understanding of the interaction mechanism between individual phonon modes and orderly moving core is of crucial importance in nanoscale tribology.

In this work, we present a phonon wave-packet simulation based study of the scattering mechanism of individual phonons in pristine CNTs, in order to elucidate their role in phononic dissipation occurring in co-axially sliding oscillators. Although, due to sliding instabilities, all phonon modes are involved to some degree in the dynamics of dissipation, here we study only those modes individually that are known to be dominant in thermal transport. High transmittance indicates less dissipation at the encounter of a single phonon and core.

II. COMPUTATIONAL DETAILS

Phonons exist over a wide range of frequencies. Low frequency phonons show a plane wave type behavior because of their long wavelength (as in the propagation of sound); whereas phonons of high frequency show a particle type behavior (as in the case of light-matter interaction). Phonon modes and other physical properties such as specific heat, dielectric,\textsuperscript{68} piezoelectric,\textsuperscript{69} elastic constants,\textsuperscript{70,71} etc., can be explained in terms of harmonic travelling waves in the atomic lattice (anharmonic forces would be required for obtaining properties such as thermal conductivity, phase transitions, etc.).

Phonon wave packet method is used in this work along with molecular dynamics simulations to study the influence of phonon scattering on the dynamics of the CNT linear oscillator. Phonon wave packet method has been used by Schelling \textit{et al.}\textsuperscript{66} to study scattering mechanism at the coherent semiconductor interface, by Refs. 64, 66, and 67 to study the influence of phonon scattering due to defects\textsuperscript{57} and functionalization\textsuperscript{64} on the thermal transport along CNTs, and by Helgee and Isacsson\textsuperscript{72} to investigate the phonon transmission across the grain boundaries in graphene. However, to our knowledge, phonon wave packet method has not been applied to study energy exchange mechanism in CNT oscillators.

The force constant matrix is obtained using the \textit{supercell method}\textsuperscript{64} in which the atoms in the unit cell are displaced one at a time (small enough displacement to maintain harmony) and resultant forces on all atoms of the supercell are computed. Fourier transform of this force-constant matrix gives the dynamical matrix, diagonalizing which results in phonon frequencies and phonon modes at a particular wave vector. The relation between frequencies and wave vector gives the dispersion relation.

Phonon wave packets are formed from the linear combination of vibrational eigenstates. To generate wavepacket with wavevector $q_0$ and centered at $z_0$, the initial displacement ($u$) and initial velocity ($v$) of the \textit{k}th base atom in \textit{l}th unit cell along the direction \textit{z}, assuming a Gaussian spread, are set as

$$u_{0k} = \frac{A}{\sqrt{m_k}} \sum_q \exp \left[ -\frac{(q - q_0)^2}{2\sigma^2} \right] e_{\text{iso}}(q) \exp (iq(z_0 - z_0)).$$
where $A$ is the wave amplitude, $\sigma$ is the broadening parameter to control width of Gaussian phonon wave packet (we choose $\sigma$ to be $2\pi/100a$ where $a$ is size of unit cell, such that the wave packet covers a width of 200 unitcells), $z_i$ is position of the $i$th unitcell, and $m_k$ is the mass of the $k$th atom. $\omega^s(q)$, $\mathbf{e}_s(q)$ are the frequency and eigenvector corresponding to polarization $s$ and the wave vector $q$.

The propagation of the wave packet thus generated on the outer CNT with its corresponding group velocity is simulated. Molecular dynamics simulations are conducted using LAMMPS. As in previous works on phonon wave packet simulations of CNTs, the polymer consistent force field (PCFF) is adopted to model the atomic interactions. As the parameters in this potential are developed using ab initio computations corresponding to 0 K, PCFF is a better choice for MD simulations involving ground state systems. All simulations are conducted in NVE ensemble with a time step of 1 fs. To ensure that anharmonic effects are completely avoided, the ground state ($\approx$0 K) configuration is completed within the simulation time. Thus, the simulation time span of a molecular dynamics run varied from 30 ps for high group velocity phonons to 300 ps for low group velocity phonons. Wave packet amplitude of 0.5 Å is used throughout all the simulations. (For a detailed sensitivity study to arrive at this 0.5 Å amplitude, see Fig. S1.78)

Fig. 1 shows the phonon dispersion plot for a (10,10) SWCNT unit cell (2.45 Å long and consisting of 40 atoms), calculated using the supercell method. Of the 120 possible phonon modes, only four are acoustic in nature, and being responsible for almost half of the thermal energy transport, are studied here in detail: the longitudinal acoustic mode (LA), one of doubly degenerate transverse acoustic mode (TA) and the twisting mode (TW), which is unique to nanotubes due to their symmetry. The remaining 116 are the optical modes; of these, two are picked up for further study on account of having the highest group velocities: the radial breathing mode (BR) which extends to most part of the frequency spectrum than any other mode, and the first order flexural optical mode (FO). A micron-long version of the same unit cell forms the outer CNT of the oscillator used in this study, as discussed next.

III. RESULTS AND DISCUSSION

The oscillator consists of an open ended 50 nm long (5,5) SWCNT core within a micron long (10,10) SWCNT outer tube. Fig. 2 shows the initial locations of the wave packet and the inner core. Along with moving cores with sliding velocities of 100 m/s and 300 m/s, we also studied stationary cores. We restrict the core velocity to 300 m/s in order to avoid resonance effects. Corresponding to each of the five phonon modes selected for study (LA, TA, TW, BR, and FO), a phonon wave packet is generated in the outer tube far away from the inner core (500 unit cells to the left of the centre) and we study how the individual phonon travels through the outer CNT, interacts with the inner nanostructure, and undergoes scattering. A typical phonon wave packet interaction process with inner core is depicted in Fig. 2 using wave packet displacement components corresponding to before, during, and after the interaction with inner core.

A. The enablers of ideal transmission

Fig. 3 shows the transmission coefficients of the five phonon modes for the oscillator system as a function of the
phonon energy. The group velocity (the slope of the dispersion plot in Fig. 1) is plotted along the axis on the right. Clearly, the TW and BR modes show near ideal transmission throughout the entire frequency range. In fact, the radial breathing mode is the most characteristic vibrational mode for CNTs and can help identify the chirality and diameter of the CNT through Raman scattering experiments. In this mode, all atoms vibrate radially in-phase and resemble the breathing effect.

Like the radial breathing mode, the twisting mode too shows near ideal transmission (0.95 and above) in almost the entire range of frequencies (Fig. 3(c)). With minimal radial displacements, atoms in this mode vibrate tangential to the surface of the CNT. Importantly, group velocity and phonon transmission (even in the presence of a vacancy defect) in the low energy region of TW mode have been found to be unaffected by the diameter of the outer CNT, which is unlike in other acoustic phonon modes. We conjecture that such diameter-independence extends to phonon transmission in the presence of inner core as well, provided the inner core maintains a stable interwall distance. BR and TW modes show ideal transmission irrespective of the sliding velocity of the core.

The TW and BR modes are the in-phase circumferential and in-phase radial/breathing displacements respectively as shown in Fig. 1. We believe that this symmetry in displacements, coupled with the rotational symmetry in the defect-free core, is responsible for the complete absence of scattering in the TW and BR modes. In contrast, a significant amount of scattering has been observed in the presence of mismatched symmetries where these TW and BR modes interact with defects or functionalizations instead of pristine inner CNT.

The three other modes—two acoustic (LA and TA) and one optical (FO)—are responsible for major part of the friction in CNT oscillators. These modes are studied in detail.
B. The dissipative modes

In case of CNTs with surface defects,
the acoustic phonon modes are known to transmit ideally near the \( \Gamma \)-point (i.e., at low wave numbers) irrespective of their group velocity, which is exactly what we see in Figs. 3(a) and 3(b) of this work. A similar behavior is also seen in phonon transmission at Si/Ge interface.\(^{82}\) As the frequency increases, however, there appears to be no consensus regarding the extent of correlation between transmission coefficient and group velocity in acoustic modes (Refs. 67, 75, and 81 as opposed to Refs. 64 and 74). Our study (Fig. 3(a)) shows negligible correlation between either \( \xi_{\text{LA}} \) or \( \xi_{\text{TA}} \) and \( v_g \) in low energy regions, but a significant positive correlation beyond the point of lowest group velocity.

The acoustic phonons with wavelengths very close to \( \Gamma \)-point are long enough to not interact with the inner nanostructure. Moving just right of the \( \Gamma \)-point, in the low energy range (5–15 meV), they are able to interact with the core and thereby lead to significant scattering (down to \( \sim 0.7 \) for LA). \( \xi_{\text{TA}} \) is even smaller than \( \xi_{\text{LA}} \) in this region, and can come down to 0.2. As one moves up the energy scale, \( \xi_{\text{LA}} \) and \( \xi_{\text{TA}} \) feature a sharper dip that is centered around the energy corresponding to the least group velocity. Finally, an ideal transmission region is realized in the high energy region (23–35 meV). The core velocity is not influencing the transmission in low energy region. In the high energy region, the transmission functions are deviating from the stationary case. In Fig. 3(a), the small dip at 25 meV in \( \xi_{\text{LA}} \) is amplified significantly for both sliding velocities. Moreover, for 300 m/s case, the amplified dip is shifted towards the low frequency. In contrast, the dip in \( \xi_{\text{TA}} \) at 18 meV (Fig. 3(b)) found evaded for moving core cases. The changes in the high frequency range transmission functions of moving cores indicate the strong interaction of high frequency phonon modes with the moving core.

Bending and wavy modes have been identified as the major source of energy dissipation in CNT oscillators.\(^{58,50,65}\) In general, TA mode vibrations would manifest as bending of CNT by transverse deformation of the tube structure. Although the role of TA phonon modes has been studied for CNT resonators,\(^{83}\) thermalization of CNTs,\(^{84}\) and thermal energy transport in CNTs with defects,\(^{67,81}\) their role in energy exchange in CNT oscillators has not be studied until now.

The optical phonon modes with low group velocity has been predicted earlier\(^{60}\) as strongly interacting modes between two CNTs. The optical phonon modes with wavelengths in the intermediate regime and having large enough group velocity are found responsible for non-Fourier heat conduction in SWCNTs. In Fig. 3, the optical modes, however, behave differently near the \( \Gamma \)-point compared to the acoustic modes. The general characteristic of optical phonons—low transmission near \( \Gamma \)-point—is displayed by both FO and BR modes (Figs. 3(d) and 3(e)). The strong scattering of optical modes near the \( \Gamma \)-point is due to their low group velocities causing them to be confined in the defective or edge region of the inner CNT. Therefore, the optical phonons of long wavelength cause substantial heat generation through electron-phonon interactions. Similar to LA and TA, \( \xi_{\text{FO}} \) also show a sharp dip in low energy region at 11 meV. The next dip at 15 meV is found shifted towards the high frequency side due to the core motion (the 100 m/s case). For higher core velocity, this dip is less pronounced. The small dip in \( \xi_{\text{BR}} \) at 110 meV corresponds to the band anticrossing region (where these BR modes mix strongly with other bands).

For dissipative modes (LA, TA, and FO), the transmission functions in the low energy region are almost unaffected by the core velocity. In the moderate energy region, transmission functions are changed significantly due to strong interaction of phonons with the moving core (\( \xi_{\text{LA}} \) in 22–28 meV, \( \xi_{\text{TA}} \) and \( \xi_{\text{FO}} \) in 13–22 meV). Similar trends have been observed in earlier studies\(^{86,87}\) at finite temperatures. We conjecture this coupling at moderate frequencies occurs due to resonance. Further, in the high energy region, the transmission functions are unaffected and all three dissipative modes transmit ideally irrespective of core velocity.

The increased scattering of slower LA phonons is well agreeing with earlier studies.\(^{75,81}\) The interface scenario in the CNT oscillator system provides a new perspective to comprehend this behavior. The severity of scattering in low group velocity region for LA phonons in our oscillator can be explained by considering both phase velocity \( v_p \) and group velocity \( v_g \) as presented in Fig. 4. However, in an earlier study by Wang and Wang,\(^{81}\) the scattering of slower LA phonons in CNTs with Stone-Wales defects (no inner core) has been investigated. Using an infinite atomic chain as simplified model, they demonstrated the correlation between low transmission and low group velocity as a general characteristic of phonon transport across CNT with broken translational invariance. Their classical acoustics based reasoning is that a low group velocity in the LA mode causes the phonon wave impedance to be low, which in turn causes slower phonons to almost completely be reflected by the defect.

From the Fig. 4, we conjecture that a high value of the ratio \( v_p/v_g \) is the reason for the huge scattering at low group velocities. In the LA mode, atoms vibrate mainly along radial and axial directions. For the duration of time when the packet passes over the inner tube, packets with the slower group velocity have a higher number of radial oscillations.

![Fig. 4. Ratio of phase velocity to group velocity, \( v_p/v_g \) (red) on right y axis; and on left y axis, phase velocity (black) and group velocity (blue) of LA mode as a function of incident phonon energy, \( h\nu \).](image-url)
This number of oscillations over the inner tube is directly correlated with \( \frac{v_p}{v_g} \). Fig. 4 clearly shows a sharp increase of \( \frac{v_p}{v_g} \) corresponding to the least group velocity.

From the results of transmission functions of five important phonon modes, we can observe ideally transmitting BR and TW modes and a narrow frequency band (5–15 meV) in which the major scattering occurs for three dissipative modes. The TA and FO modes show a severe scattering in this frequency band. The sliding velocity significantly modifying the transmission functions of all three dissipative modes, however, not in the peak scattering region.

**C. Dynamics of the scattering events**

Further, to elucidate the frictional dissipation mechanism, we now look at the scattering events created as a phonon wave packet travels along the outer tube of the oscillator and encounters the inner core. In each case, the excitation starts at 500 unit cells left of the center of the stationary core and travels right. Fig. 5 shows the time evolution of kinetic energy along the length of the oscillator (taken to be the kinetic energy of the first basis atom of each unit cell). The top row corresponds to the LA phonons, the second row to the TA phonons, and the last row to the FO phonons. In each of these nine panels, the square plot corresponds to energy time history of the outer CNT while the companion strip corresponds to the core. It should be noted that the color scales corresponding to the nine panels are all different.

Phonons with three different energies are studied for each mode. For the LA mode, we choose three phonons (5.76, 9.18, and 12.3 meV) that outline the profile of the first dip in the transmission plot occurring to the right of the...
gamma point in Fig. 3(a). For the TA mode, we choose one close to the gamma point (2.4 meV), one at the first dip (8.15 meV), and one near the lowest $v_g$ (17.76 meV) in the transmission plot (Fig. 3(b)). For the FO mode, we again choose three phonons (8.78 meV, 11.3 meV, and 13.54 meV) that outline the profile of the first dip in the transmission plot (Fig. 3(c)). Although these three modes are responsible for energy dissipation in CNT oscillators, each mode has its own characteristic behaviour distinctly different from the other two.

In the LA mode, the wave packet creates the first scattering event in the outer tube only when it travels over the right end of the core. A substantial part of the packet is reflected back first through the inner CNT, part of which then is sent back along the outer CNT as it reaches the left end of the core. This creates a cycle of slowly decaying scattering events and represents anomalous reflection of LA phonon by the inner core.

Although the two dips in the transmission function are very similar to those in the LA mode, the scattering events in the TA mode are significantly different from those in LA.

The packet starts at 500 unit cells to the left of the centre as before. While the long wavelength TA phonon shows no scattering (Fig. 5(d)) as it passes over the core, the one near low $v_g$ shows diffused scattering (Fig. 5(f)). For the TA phonon with energy near the first dip (middle panel), scattering occurs as soon as the packet reaches the left end of the core, whereas for the LA phonon with the same energy profile, scattering occurs only when the packet has travelled the length of the core.

The first order optical phonons too behave very differently from the LA mode. Not only is there a substantial reflection as soon as the phonon encounters the inner core, but also when the phonon passes over the right end of the core. The diffused scattering however in the right panel is similar to that observed for TA phonons with the lowest group velocity.

Similar to the TW and BR modes, the LA mode also has rotational symmetry in match with the symmetry of inner CNT. Surprisingly, the LA mode is not showing ideal transmission. From the scattering events (Figs. 5(a)-5(c)), first we can observe the unscattered passage of the LA mode phonon wave packet over the left end atoms of inner CNT which is similar to the TW and BR modes. Afterwards, the dominated longitudinal component of the LA mode wave packet causes an intense shearing that leads to transmission of wave packet energy into inner CNT. The transmitted part of wave packet continues to propagate in the inner CNT and causes an end scattering due to right end atoms. The reflected part of wave packet propagates towards left end while part of its energy transmitting to the outer CNT. This oscillating decay of the LA mode wave packet in the core, which can be clearly seen in the contour strips corresponding to the inner core.

For the TA and FO modes, such a matching symmetry does not exist. Once the propagating phonon encounters the mismatched symmetry or augmented degrees of freedom due to the presence of inner CNT (at the ends itself), it generates quasibound vibrational states in the inner CNT. The generated low quasibound state acts as localized scatterer and causes mixing of modes and severe scattering. From the trends of TA and FO modes, we can predict the dissipation due to other unstudied optical modes is in proportion with their transverse atomic displacements. The BR and TW modes are found to display near ideal transmission irrespective of the sliding velocity which indicates that the phonon vibrational modes with matched symmetry with core (unlike dissipative modes) causes no scattering. Hence, such phonon modes can be recognized as the enablers of ultra-low dissipation in coaxial sliding of CNTs.

IV. CONCLUSIONS

We have studied single mode phonon scattering dynamics in co-axially sliding CNTs. The radial breathing and twisting modes (which are relatively high group velocity phonons) are potentially the major contributors to ultra-low friction in CNT oscillators. Over a wide range of frequencies and for core velocities up to moderate values (~300 m/s), they show near ideal transmission. Extensive testing with wavepacket amplitudes in the feasible range (0.1–1 Å) confirmed that the BR mode’s ideal transmission is not affected by wavepacket amplitude.

In contrast, the major participants in phonon dissipation in CNT oscillators are two acoustic (longitudinal and transverse) and one optical (first order) modes. We found the energy ranges of phonons that can prevent ideally smooth sliding of CNTs. The transmission plot in the LA mode features two dips, and the first one (at low phonon energies, in the 5–15 meV range) is characteristic of the core. The maximum scattering observed in the TA mode (~0.9) is higher than that in the LA mode (~0.5), which suggests the dominance of out of plane deformations in the damping of oscillations. An anomalous reflection of LA phonon is observed. Up to moderate velocities of the moving core (up to 300 m/s), the essential scattering behavior in the LA, TA, and FO modes is not changed; however, an amplification or suppression of few high frequency modes is observed due to the moving core.

We restricted the core velocity to a moderate value of 300 m/s in this work since at very high core velocities (between 800 and 1100 m/s), we found the BR mode of the outer CNT to become excited (not shown in this paper) similar to other works. We conjecture that such high amplitude resonance in the BR mode engenders LA phonons, which in turn causes a high frictional dissipation.

Although the present simulations are conducted on a ground state configuration, the deformations imposed by the thermal effects, wavy and sagging deformations of long CNTs (which essentially create the out of plane deformation on the walls of outer CNT) causes further scattering. Thus, the dissipation behavior could be affected by the deformations due to structural instabilities. Since the anharmonic effects indulge in observing single mode wave packet, studying finite temperature scattering behavior of single mode phonons is not possible. However, the present trends, in essence, corroborating the previous MD simulations based results.
In this study, we restricted the core geometry to an uncapped (5,5) CNT of 50 nm long. Our future work will address the effect of core geometry in detail by considering different core structures. Preliminary results suggest that a certain amount of core geometry dependence may exist on phonon scattering dynamics. For example, when the length of open ended (5,5) CNT is doubled the first dip in the LA transmission mode appears to shift towards the Γ-point and the corresponding phonon scattering increases in magnitude. Also, when the armchair CNT is replaced by a zigzag CNT of almost the same diameter, the first dip in LA transmission appears to become more pronounced indicating an increased of almost the same diameter, the first dip in LA transmission appears to become more pronounced indicating an increased scattering by the zigzag core. Preliminary results also appear to suggest the exciting possibility that the transmission plot can be used to identify the inner core structure using its unique signature.

Our findings may lead to better design of sliding surfaces and to make highly efficient functional devices. Being able to drive or cool specific phonon modes in order to control individual phonons in situ is a promising way to engineer the performance of CNT coaxial oscillators. However, controlling individual phonons in situ remains extremely challenging.

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(Refer to the original text for all the numbered references and citation details.)