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Trans-phonon effects in ultra-fast nanodevices

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Abstract

We report a novel phenomenon in carbon nanotube based ultra-fast mechanical devices, the trans-phonon effect, which resembles the transonic effects in aerodynamics. It is caused by dissipative resonance of nanotube phonons similar to the radial breathing mode, and subsequent drastic surge of the dragging force on the sliding tube, and multiple phonon barriers are encountered as the intertube sliding velocity reaches critical values. It is found that the trans-phonon effects can be tuned by applying geometric constraints or varying chirality combinations of the nanotubes.

Supplementary data are available from stacks.iop.org/Nano/19/255705

(Some figures in this article are in colour only in the electronic version)
In MWNT oscillators driven by the van der Waals restoring force between the coaxial cylindrical graphene shells, relative axial speeds between the core and the sheath can reach as high as 1400 m s\(^{-1}\) [7]. For such a ultra-fast nanodevice, if and how sliding energies dissipate into heat constitute some of the intriguing questions. Previous studies show that in the double-walled carbon nanotubes (DWNTs) spanning no less than several nanometers, energy dissipation occurs quickly and axial oscillation vanishes in a few nanoseconds. Internal mechanical modes of the graphene shells are excited by sliding motion [3] and energy conversion is found to be velocity-dependent [7] and nonlinear when the axial speed exceeds a critical value [9]. For instance, Servantie and Gaspard [9] have extracted, from their simulation results, a relation between the friction and the maximum translation velocity of the oscillating tube, and they have reported a transition of the friction–velocity relation from linear to nonlinear at a ‘critical velocity’, suggesting the onset of additional dissipating mechanisms that may ‘involve the breathing motion of the nanotubes’. Furthermore Tangney et al, found that the friction force in sliding carbon nanotubes can be significantly enhanced when phonons whose group velocity is close to the sliding velocity of the nanotubes are strongly excited [18]. However, much remains to be understood with regard to dynamic energy transfer channels in the MWNT oscillators. To this end, we perform a molecular dynamics study of a pair of armchair carbon nanotubes (7, 7)@(12, 12) via the GROMACS package [19]. In the simulation with time step 1 fs, the Dreiding force field [20] is employed to describe the intratube covalent and intertube van der Waals interactions. Periodic boundary conditions with a 5.1 nm supercell are used to simulate an infinite tube length. Furthermore, one carbon atom in the outer tube is fixed axially to retain the relative motion of different graphene shells.

After structural relaxation, various axial velocities \(V_0\), ranging from 100 to 2000 m s\(^{-1}\), are assigned to the inner tube. The axial intertube speed, plotted in figure 1(A) as a function of time, is found to be mostly dependent on the tube. The axial intertube speed, similar to the onset of sliding friction in the one-dimensional Frenkel–Kontorova model [15]. In figure 1(B) we plot the axial force dragging on the inner tube (\(V_0 = 1000\) m s\(^{-1}\)) versus time. At \(t = 4700\) ps the dragging force on the inner tube experiences a sudden surge. Further analysis shows that the surge of the dragging force is caused by large deformation of the tube walls. The phenomenon bears a resemblance to the transonic effects that had caused drastic reductions of the forces lifting early airplanes in the catastrophic events. Below or above a critical speed range (CSR), the friction is very small while as the speed falls into a CSR the friction is drastically amplified by several orders of magnitudes. A CSR serves as a ‘barrier’ for

\[
V_0 = 1000, 1100, 1900 \text{ m s}^{-1}
\]

Sudden drops of the axial speed are found when the speed falls into the CSRs centered at 540 (see the inset), 930, 1080 and 1870 m s\(^{-1}\), respectively. The time/speed span for the inset are 5 ns and 1.2 m s\(^{-1}\). Between CSRs the axial speeds have little slow-down within 5 ns. (B) The dragging force on the inner tube versus time. The initial speed of the tube \(V_0\) is 1000 m s\(^{-1}\). The force is calculated by differentiating the velocities with averaging over 10 ps.

\[
\begin{align*}
\text{CSR} & \to 540, 930, 1080, 1870 \text{ m s}^{-1} \\
V_0 & \to 1000, 1100, 1900 \text{ m s}^{-1}
\end{align*}
\]

Figure 1. (A) Time evolution of the axial speed of the inner tube with various initial speeds \(V_0\) ranging from 100 to 2000 m s\(^{-1}\). Sudden drops of the axial speed are found when the speed falls into the CSRs at 540 (see the inset), 930, 1080 and 1870 m s\(^{-1}\), respectively. The time/speed span for the inset are 5 ns and 1.2 m s\(^{-1}\). Between CSRs the axial speeds have little slow-down within 5 ns. (B) The dragging force on the inner tube versus time. The initial speed of the tube \(V_0\) is 1000 m s\(^{-1}\). The force is calculated by differentiating the velocities with averaging over 10 ps.
the inner tube to pass through, and we term it as a ‘phonon barrier’. Unlike the transonic phenomenon with one sonic barrier, the inner tube has several phonon barriers. The overall phenomenon is hence named as the trans-phonon effect due to its resemblance to the transonic effect.

To gain further insight into the catastrophic event, principal component analysis (PCA) [22] has been performed for the atomic trajectories \( x_i(t), t = 1, \ldots, 3N \), for the first 500 ps, where \( N \) is the total number of atoms. Eigenvalues of the covariance matrix \( C_{ij} = \langle (x_i - \langle x_i \rangle)(x_j - \langle x_j \rangle) \rangle \) measure contributions of corresponding principal modes, where \( \langle \cdot \cdot \cdot \rangle \) denotes the time average. The eigenmodes are average translational, rotational, vibrational modes, or various non-rigid-body modes of the trajectory. We plot in figure 2(A) the eigenvalues for the leading 50 principal modes with respect to various initial speeds. In all these cases the translational mode (indexed as ‘1’ in figure 2(A) has the largest contribution to the dynamical motion of the system, followed by the intertube rotation (indexed as ‘2’) whose contribution is one to two orders of magnitude smaller. One can see from figure 2(A) that contributions from non-rigid-body modes (indexed as ‘3’ and above) are negligible when the axial speed \( V \) is outside the CSRs. However, for speeds within the CSRs such as \( V_0 = 1000 \text{ m s}^{-1} \), many non-rigid modes have been excited. PCA has been carried out for \( V_0 = 1000 \text{ m s}^{-1} \) at several simulation time intervals to reveal the progressive excitations. The RBM-like modes are excited within the first 100 ps and reach their saturation at \( \sim 500 \) ps. Translational energies in the inner tube are then dissipated slowly into higher-frequency modes prior to the sudden drop of their sliding speed at \( 4700 \) ps. The carbon atoms on the tubes are displaced violently from their equilibrium positions \( t = 4700 \) ps, which leads to a huge increase in the dragging force on the sliding tube. This result shows that, within the CSRs, the RBMs are excited via resonance followed by the excitations of higher-frequency modes. Figure 2(A) reveals the passage of successive excitations of the RBMs and other modes when the sliding speed is within one of the CSRs. Here the resonances are caused by the internal mode couplings, and are thus not the conventional parametric resonances [23]. However, the resonance of the RBM-like modes alone is not sufficient to cause the trans-phonon phenomenon. The large deformation of the tube walls that follows the resonance of the RBMs is directly responsible for the surge of the dragging force and thus the occurrence of the trans-phonon phenomenon.

To examine the excited modes in detail, we have calculated \( p_j(t) = x(t) \cdot u_j \), which are projections of the atomic trajectory \( x(t) \) onto the leading principal modes \( u_j \). As shown in figures 2(B)–(F), the non-rigid mode that has the largest contribution is the RBM followed by the wavy modes [3]. After they are mostly excited after \( t = 500 \) ps, the RBMs are enhanced by about one hundred times compared with their earlier amplitudes (figure 2(E)). Furthermore, many high-energy modes are excited (figure 2(A)) due to their couplings with the RBM [15], leading to irreversible energy dissipation. Similar behavior has been observed in other CSRs, such as \( V_0 = 1100 \) and 1900 m s\(^{-1}\).

Inspired from the above observations, we propose two means to avoid or reduce the trans-phonon effects for any given carbon nanotube. One is to reinforce the nanotunnel to elevate the RBM frequencies to a level higher than the WBFs. For that purpose, we fix in space carbon atoms in the outer tube and perform the simulation under such a constraint. In figure 3 we plot its axial speed as a function of time. Due to suppression of its coupling to the RBMs after immobilizing atoms in the outer tube, the axial speed hardly decreases with time. Similar observations have been made previously for DWNT oscillators in which atomic coordinates in the outer tube are fixed to prevent the formation of nanotube wavy motion during dynamics simulation [3, 4]. In practice, multi-walled carbon nanotubes can be used to achieve the constraint: our simulation of a triple-walled nanotube (TWNT)
Since phonon phenomenon is not observed in the first 5000 ps. outside the CSRs as compared to those at low temperatures. larger energy losses are observed when the sliding speed is out and similar trans-phonon behavior is found, albeit much the CSRs before (after) the steep drops in speed. Simulations versus time for double-walled systems (12, 0)@(21, 0) and (11, 2)@(12, 12) of the first. In figure 3 we also plot the axial speeds of the second and third DWNTs for a given speed are reduced by factors of 1.7 and 6.9, respectively, compared with those (black solid). Two methods: (i) elevating RBFs by applying constraints on the outer tube (gray dashed) and (ii) reducing WBFs by using chiral tubes (11, 2)@(12, 12) have effectively avoided the severe energy dissipation due to resonant coupling with radial breathing phonons (red dashed). The time/speed spans for the detailed data shown in the inset are 100 ps and 0.7 m s\(^{-1}\) separately. (7, 7)@(12, 12)@(17, 17) confirms the suppression due to the confinement of the outermost tube (17, 17). It was found that the RBM frequencies, either in-phase or out-of-phase, of DWNTs are nearly independent of tube chiralities and follow approximately a power-law relation \(\sim c/D\) on outer tube diameters \(D\) [21]. This suggests another means to alleviate axial speed losses by choosing the desired combinations (or chiralities) of nanotubes that make up the DWNT to reduce the WBFs to a level lower than the RBM frequencies.

DWNTs (7, 7)@(12, 12), (12, 0)@(21, 0) and (11, 2)@(12, 12), for example, have similar diameters and are all commensurate pairs but with different commensurate lengths 0.246, 0.426 and 1.7 nm, respectively. Thus the WBFs of the second and third DWNTs for a given speed are reduced by factors of 1.7 and 6.9, respectively, compared with those of the first. In figure 3 we also plot the axial speeds of the double-walled systems (12, 0)@(21, 0) and (11, 2)@(12, 12) versus time for \(V_0 = 1000\) m s\(^{-1}\). As expected, the trans-phonon phenomenon is not observed in the first 5000 ps. Since \(V_0 = 1700\) m s\(^{-1}\) falls into one of the CSRs of the (12, 0)@(21, 0), all characteristics of the trans-phonon effects become evident (see figure S1 in supporting material (available at stacks.iop.org/Nano/19/255705)). Finally, using smaller DWNTs is another effective means for avoiding the excitation of RBMs because smaller DWNTs have higher RBMs, as implied by the observation of Servantie and Gaspard [9].

Molecular dynamics simulations performed so far are all conducted with an initial temperature 0 K, and the energy dissipation that follows heats up the nanotubes to \(\sim 5\) K if \(V_0\) is outside the CSRs, and to \(\sim 20\) K (30–50 K) if \(V_0\) is inside the CSRs before (after) the steep drops in speed. Simulations at room temperatures (e.g. 300 K) have also been carried out and similar trans-phonon behavior is found, albeit much larger energy losses are observed when the sliding speed is outside the CSRs as compared to those at low temperatures.

Furthermore this thermally induced dissipation is found to be velocity-independent. In addition, we have also carried out simulations with different supercell lengths, e.g. 7.5 and 10 nm, and found that the wavy mode depends upon the length [3, 7]. This dependence, as our simulation shows, affects the coupling strengths among the RBM, wavy and axial sliding modes, but leaving unchanged other characteristics of the trans-phonon phenomenon (e.g. the sudden drop of the sliding speed, the significant deformation of radial motion and the surge in the dragging force). These results are presented in the supporting material (available at stacks.iop.org/Nano/19/255705).

To conclude, the trans-phonon phenomenon is found to be mainly responsible for energy dissipation in an ultra-fast nanoscale mechanical system composed of MWNTs. In addition to dissipation mechanisms previously identified for DWNT oscillators, such as the rocking motion instability or the end effects [3, 7, 8], the trans-phonon behavior is primarily due to resonant coupling of the axial motion to a wide window of phonon modes and the subsequent giant deformation of the tube walls. Multiple phonon barriers are discovered as the intertube velocities reach resonant values that are determined by the DWNT diameter and commensurate length as well as diameter. The results reported here are believed to have important implications for ultra-fast nanodevices in general that possess phonon frequencies prone to velocity-induced resonances of moving parts. Moreover the means to reduce energy losses proposed here will have wide applications in NEMS design.

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References

[10] Craighead H G 2000 Science 290 1532