Intrinsic Energy Loss Mechanisms in a Cantilevered Carbon Nanotube Beam Oscillator

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Classical molecular dynamics is applied to study the energy dissipation (the Q factor) of the cantilever-type beam oscillators of single wall and double-walled carbon nanotubes (CNTs). The study finds that the Q factor of the CNT beam oscillator varies with the temperature T following the $1/T^{0.36}$ dependence. For single wall CNT, the Q factor drops from 2×10^5 at 0.05 K to 1.5×10^3 at 293 K. The study further reveals that the weak interlayer binding strength and the interlayer commensurance significantly increases the energy dissipation in the double-walled CNT oscillator.

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Carbon nanotubes (CNT) exhibit appealing properties, such as extremely high in-plane elastic modulus and thermal conductivity. These properties, combined with their nanometer-sized and perfect atomic structure, imply potential applications of CNT in nanoelectromechanical systems as components for high frequency oscillators for sensing and signal processing applications [1,2]. For example, Poncharal et al. [1] demonstrated the use of the resonance of a cantilevered CNT to estimate the mass of an attached carbonaceous particle as light as 30 fg inside a transmission electron microscope.

The sensitivity of a mechanical beam oscillator, which usually operates at its harmonic resonance frequency in practical applications, depends mainly on the quality factor Q (the inverse of the energy dissipation) of the oscillator. Here Q is defined as the ratio of the energy stored to the energy dissipated by losses in the oscillator. However, the Q factor and the associated energy loss mechanism of CNT beam oscillators have not been studied, and a high Q factor CNT oscillator has not been realized. The highest Q factor ever reported from the experimental studies using cantilevered multiwalled CNTs ($\sim$20 nm in diameter) reaches only $\sim$1000 at room temperature and in a vacuum [1,3]. In contrast, oscillators with Q factor in the order of 10^5 or higher at a low temperature around 100 mK have been demonstrated with Si or diamond beams a few hundred nanometers long [4].

In order to investigate the energy dissipation mechanisms and to determine the theoretical limit of the intrinsic Q factor of a CNT beam oscillator, we apply the classical molecular dynamics (MD) method in the following to model the oscillation behavior of CNT. Carbon atoms that form covalent bonds on CNT are modeled with a second-generation many-body Brenner potential [5]. The potential is an extension of the Tersoff-Brenner potential [6] to allow for covalent bond breaking and forming, including the associated changes in atomic hybridization within a classical potential. The potential reproduces accurately the binding energy, the lattice constants, and the elastic constants of CNT.

Figure 1 shows schematically a CNT model for the computation. Carbon atoms at one end of the CNT are fixed. After an initial equilibration at a finite temperature, the CNT is subject to a point bending force at the free end and deflected to a certain displacement as shown in Fig. 1. Upon the removal of the bending force, the CNT is left to oscillate freely. In the computation, a constant energy condition is imposed (i.e., a microcanonical ensemble, in which the number of molecules, the volume and the total energy, are kept constant) during the free oscillation. This is enforced by requiring the variation of the total system energy (which should be constant) in the computation to be less than 0.03% of the external potential energy E_{ext}. E_{ext} is the difference of the total energy before and after the deflection of the free end of the CNT beam. The time step in the MD simulation is 10^{-15} s.

The cyclic oscillation of the CNT is accompanied by the cyclic conversion between the potential energy and the kinetic energy of the oscillator. The maximum external potential energy, however, is reduced to $E_{\text{ext}} - \Delta E_{\text{ext}}$

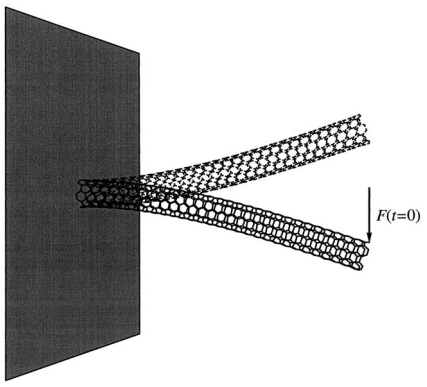

FIG. 1. A schematic showing a single wall carbon nanotube beam oscillator for modeling.

at the end of each oscillation cycle due to energy loss or damping, where ΔE_{ext} represents the energy loss in each oscillation cycle. The Q factor is thus defined as $Q = 2\pi E_{\text{ext}}/\Delta E_{\text{ext}}$. At the end of n cycles, the maximum external potential energy E_n is related to the initial maximum potential energy E_{ext}, by $E_n = E_{\text{ext}}(1 - 2\pi/Q)^n$, if Q is assumed constant.

We begin with a (5, 5) single wall CNT (SWCNT) that has 240 carbon atoms and is about 3 nm long. The initial displacement of the free end of the CNT (Fig. 1) is set at 0.3 nm, a small enough displacement to avoid significant deformation in CNT. Figure 2 shows the external potential energy versus time for the resulted oscillation of the SWCNT. The initial temperature, which is defined according to the internal energy of the system, is 8 K prior to the bending force, and it rises slightly after the bending force is applied. The figure shows 88 cycles in 300 ps. The gradual decrease of the external potential energy due to the energy loss in the oscillation is obvious. The insets in Fig. 2 show the oscillation amplitude at the free end of the CNT in the time interval of 0–10 ps and 290–300 ps. The comparison of the two inset plots shows that the magnitude of vibration decreases, while the oscillation frequency is constant as expected.

The dissipation of the external potential energy during the oscillation resulted in the rise of the internal energy; i.e., part of the potential energy is converted into internal energy. Figure 3(a) shows the internal energy of the CNT at the peak of each oscillation cycle. The dashed line represents a linear fit of the data. The internal energy, thus the temperature, increases gradually with time, even though this increase is not exactly monotonic. This temperature increase is quantitatively consistent with the loss of external potential energy shown in Fig. 2.

The sensitivity of the Q factor to the initial nanotube beam deflection is also examined. At the initial temperature of 8 K, the Q factor values of the oscillator are 6810 and 6870 for the initially imposed bending displacement of 0.3 nm and 0.2 nm, respectively. The initial oscillation amplitude thus does not obviously influence the Q factor.

Varying the temperature of the system in the modeling reveals the temperature dependence of the Q factor. The initial temperature T of the system is varied from 50 mK to 293 K. As shown in the logarithmic plot of Fig. 3(b), the Q factor drops from 2×10^5 at 50 mK to 1.5×10^3 at the room temperature. The dependence between Q and T can be fit with $Q \propto 1/T^{0.36}$, which deviates from the classic $1/T$ dependence for ideal regular-sized beam oscillators. This deviation will be discussed later.

We now turn to modeling the oscillation double-walled CNT (DWCNT), representative of multiwalled CNTs. It is expected that new energy dissipation mechanisms could be introduced in a DWCNT beam oscillator due to its different mechanical structure compared to SWCNT. In the modeling, the interlayer interaction in DWCNT is characterized by the van der Waals potential for carbon [7]. Two types of DWCNTs are modeled, a (5, 5)/(18, 0) one possessing an incommensurate interlayer lattice matching, and a (5, 5)/(10, 10) one having a commensurate interlayer lattice matching.

The interlayer spacing in a (5, 5)/(18, 0) DWCNT is established to be 0.36 nm. The length of the DWCNT is chosen to be ~3 nm. The DWCNT is then set to oscillate with an initial temperature of 8 K. Figure 4(a) shows the change of the external potential energy with time, which reveals that the energy dissipates much faster than that in the SWCNT. The Q factor for this DWCNT is calculated to be 1270, much smaller than that ($Q = 6810$) for the SWCNT modeled previously at the same temperature,

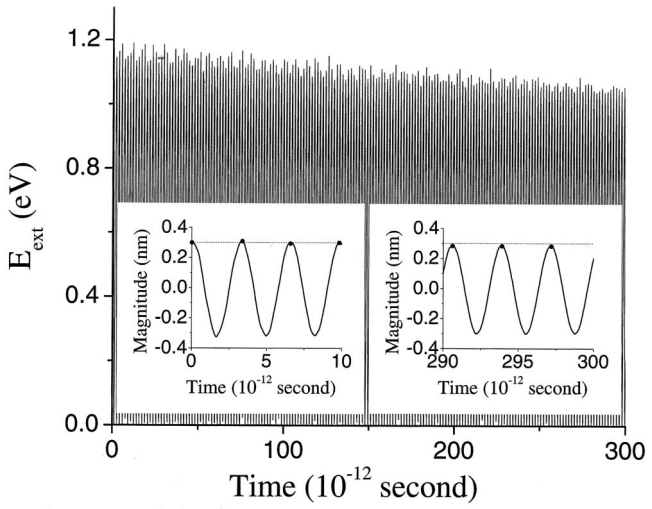

FIG. 2. The external potential energy E_{ext} versus time for the oscillation of a (5, 5) single wall carbon nanotube at an initial temperature of 8 K. The insets show the oscillation amplitude at the free end of the carbon nanotube versus time in the time interval of 0–10 ps and 290–300 ps.

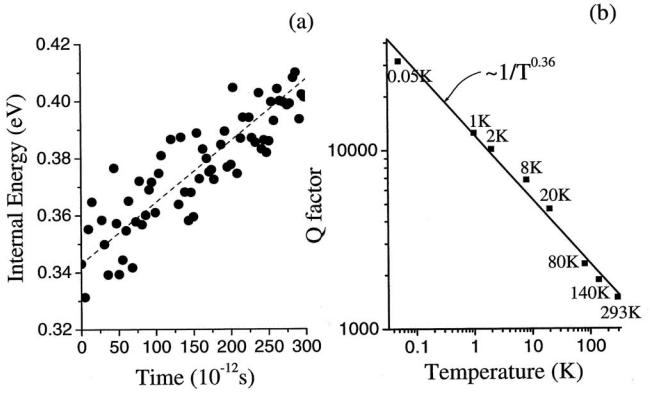

FIG. 3. (a) The internal energy of the nanotube at the peak of its oscillation versus time from the same calculation shown in Fig. 2. (b) The quality factor Q versus temperature dependence for a (5, 5) single wall carbon nanotube.

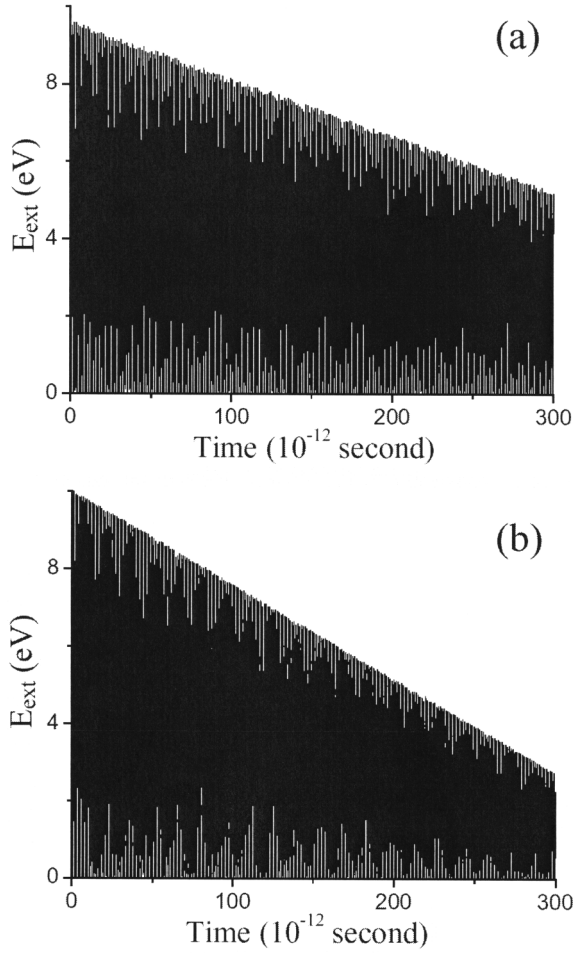

FIG. 4. The external potential energy E_{ext} versus time for the oscillations of a (5, 5)/(18, 0) double-walled carbon nanotube (a), and a (5, 5)/(10, 10) double-walled carbon nanotube (b), at an initial temperature of 8 K.

though the calculated Q factor is still in the same order of the experimentally measured Q factor for multiwalled CNT beam oscillators [1,3]. In contrast, Fig. 4(b) shows the result for a similar-sized DWCNT (5, 5)/(10, 10) modeled under the same initial conditions. The dissipation of external potential energy occurs even faster. The Q factor calculated for such a commensurate DWCNT is only 650, half of that for the incommensurate (5, 5)/(18, 0) DWCNT.

The result indicates that the interlayer interaction introduces new energy dissipation venues in DWCNT beam oscillators, and in addition to that, interlayer lattice matching also plays a noticeable role. Recent experimental [8] and theoretical studies [9] on multiwalled CNTs concluded that though the resistance to the interlayer sliding is minimal due to the weak van der Waals interlayer interaction, the interlayer binding energy and the interlayer sliding resistance are relatively higher between commensurate layers than between incommensurate layers.

To further elucidate the role of the interlayer binding strength on the energy dissipation in DWCNT, we model the oscillation of the same (5, 5)/(18, 0) DWCNT at 8 K, but use a fictitious interlayer interaction force that is 10 000 times higher than the actual van der Waals forces. The resulted interlayer interaction is thus comparable to the covalent bond strength of carbon. The calculated Q factor for such a DWCNT is 7600, which is nearly 6 times higher than that of the same DWCNT previously studied, but comparable to that of the SWCNT. The result confirms that the weak interlayer binding strength contributes significantly to the energy dissipation in DWCNT.

The sixfold increase in energy dissipation simply due to the weak interlayer binding strength and the additional twofold increase due to the interlayer lattice matching in DWCNT in our modeling point to the existence of significant damping mechanisms intrinsic to the structure of such nanotubes. Such damping mechanisms coupled with the rippling mode induced damping [1,10] existed only in thick walled CNT are responsible for the experimentally measured low Q factor for multiwalled CNT beam oscillators.

The study indicates that there exist significant internal energy loss mechanisms for CNT beam oscillators. For SWCNT, even though it has a high in-plane elastic modulus and thus high tensile rigidity, the rigidity in the lateral direction (perpendicular to the CNT axial direction) is significantly less [11]. Such a reduced rigidity in the lateral direction, however, is responsible for the bending deformation associated with the beam oscillation [12]. The same argument applies also to multiwalled CNT, which, nevertheless, consists of weakly coupled nested CNT layers. It is known that the thermoelastic energy loss mechanism at high temperature (>100 K) is more pronounced in a thin-beamed oscillator involving bending deformation [12,13]. The classic description of thermoelastic loss in the flexure deformation of an isotropic crystalline beam [12,13] follows: $Q^{-1} = \frac{E\alpha^2 T}{c}\omega\tau$ for $\omega\tau \ll 1$, where E is the Young's modulus, α is the coefficient of thermal expansion, c is the specific heat, T is the temperature, ω is the oscillation frequency, and τ is the thermal relaxation time. $\tau = a^2 c/\pi^2 k$, where a is the beam thickness and k is the thermal conductivity. It predicts the decrease of Q with the increase of temperature, which is consistent with the trend shown in Fig. 3(b) for the SWNT. However, the $Q \propto 1/T^{0.36}$ dependence obtained for SWCNT from the modeling presents a deviation, and manifests the importance of size and structure of beam oscillators at the nanoscale. The result is consistent with other experimental studies on the energy losses in microscale or nanoscale beam oscillators. For example, Mohanty et al. [14] have observed a $1/T^{0.25}$ dependence of the Q factor for single crystalline Si and GaAs oscillators at temperatures below 40 K, though the exact origin of such dependence has not yet been revealed.

The similarity in the $Q - T$ dependence is extremely intriguing considering the significant structural difference between SWCNT and other studied Si or GaAs crystalline beams. It may simply imply that there exists a general energy loss mechanism for nanoscale-sized structures. For Si and other crystalline structures, low energy defects, such as shallow semiconductor donors or acceptors, point defects and other complex defects due to lattice distortion are usually considered as the involved two-level systems (TLS) in the energy dissipation. In the classic TLS theory, energy dissipation is described as the dispersion and absorption of the elastic wave through the TLS/elastic wave coupling and through the phonon exchange processes. However, for the studied CNTs, which are modeled as having perfect lattice structure in their bulk, the related defects may consist of mainly the distorted lattices at the edges of the open ends. In the study of energy dissipation in crystalline Si oscillators at low temperature, Mohanty et al. [14] speculate that the configurational entropy of a large number of degenerated TLS states and the high operating frequency of the oscillator may be, respectively, responsible for the increase and the lack of temperature dependence in energy dissipation; and propose that the coupling between the TLS and the phonons can be quantum mechanically modeled as the tunneling of the localized phonons between the split energy levels. A recent theory [15] indeed applied such a quantum mechanics approach, and revealed that a phonon pumping process in TLS defects could explain the weak temperature dependence of energy dissipation in microscale and nanoscale structures. Because of the small size of nanoscale oscillators compared to the wavelength of the participating phonons, the collective participation of the TLS defects in the relaxation and energy dissipation of the oscillator is required. Such a collective effect leads to an enhanced and correlated phonon emission (the super radiance), which can then contribute to large energy dissipation [15]. For the studied CNT, which has a diameter of around 0.7 nm and a length of 3 nm, significant energy dissipation through the aforementioned mechanism is very plausible; and the defects consisting of the C structures around the open ends of CNT should be able to serve as TLS scattering centers.

Another intriguing result obtained from this study is the persistent weak temperature dependence of energy dissipation up to room temperature [as shown in Fig. 3(b)], different from that observed in other types of single crystalline beams. This shows such weak temperature dependence only at cryogenic temperature [14]. The difference could be due to the much higher oscillating frequency of the studied CNT resonators (up to several hundred GHz) and the expected stronger phonon-TLS coupling in such CNT systems [15].

The relatively low Q factor for CNT beam oscillators revealed in this study, which is intrinsic to the structure of CNT, is disadvantageous, especially, for its applications in high sensitivity resonance sensing. However, other unique properties of CNT, such as its small dimension, size uniformity, high thermal conductivity, and chemical inertness, could be taken advantage of in the design of new CNT electromechanical devices. Because of the general limitation of atomistic modeling in extracting directly some physics-related parameters, further theoretical and experimental studies of the effect of size, defect, clamping condition, and environment on the CNT beam oscillator operation are also called for, which could lead to better understanding of the energy loss mechanism in nanoscale oscillators.

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