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Mechanics of thermophoretic and thermally induced edge forces in carbon nanotube nanodevices

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ABSTRACT

A double walled carbon nanotube thermal actuator consisting of a short outer tube sliding along a long inner tube under a temperature gradient is used as a model system to investigate the mechanics of thermophoretic and thermally induced edge forces in nanoscale contact based on the theory of lattice dynamics. It is shown that the total thermophoretic force has two components: a gradient force due to the change in van der Waals energy in the direction of temperature gradient and an unbalanced edge force due to the temperature difference between the two tube ends. Closed-form analytical expressions are derived for the gradient and unbalanced edge forces, with results in excellent agreement with molecular dynamics simulations. This study represents a first analytical study of thermophoretic and thermally induced edge forces between two solid bodies, and may have far reaching implications on thermomechanical nanodevices and nanoscale contact.

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1. Introduction

Nanoscale devices that convert various forms of energy into mechanical motion are of great interest due to many potential applications ranging from artificial muscles to data storage (Craighead, 2000; Ekinci, 2005; Ekinci and Roukes, 2005; Roukes, 2001; Rueckes et al., 2000). Since their discovery by lijima (1991), carbon nanotubes (CNTs) have been widely studied as potential building blocks for nanoscale devices because of their extraordinary electrical, mechanical, chemical, and thermal properties such as their low density, high stiffness, high strength, chemical inertness, metallic and semiconducting electronic properties, etc. (Dresselhaus et al., 1995; Popov, 2004). The one dimensional tubular shape and multi-shell structure of CNTs make them particularly suitable for devices involving rotation and translation (Barreiro et al., 2008; Cumings and Zettl, 2000; Fennimore et al., 2003). Indeed, the past decade has witnessed the emergence of a large number of nanotube-based devices, including nanomotors (Fennimore et al., 2004), gigahertz oscillators (Zheng and Jiang, 2002), memory devices (Rueckes et al., 2000), electron windmills (Bailey et al., 2008), nanoguns (Chang, 2008), and nano heat engines (Chang and Guo, 2010).

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While electric energy has been by far the most frequently used energy source in nanodevices, it has been recently shown that thermal energy can drive CNT based nanoactuators (Barreiro et al., 2008; Chang and Guo, 2010; Hou et al., 2009; Longhurst and Quirke, 2007; Schoen et al., 2006; Shenai et al., 2011; Zhao et al., 2010). A particularly interesting experiment demonstrated that thermal gradient is capable of moving nanoscale objects attached to the outer layer of a CNT in the direction of decreasing temperature (Barreiro et al., 2008). In this experiment, the authors constructed a motor consisting of a short outer carbon nanotube, to which a metal plate is attached, and a long inner carbon nanotube which is connected to two gold electrodes. An electric current passing through the inner tube causes the outer tube to move together with the metal plate. To identify the driving mechanism of the actuator, the authors showed that the metal plate continues to move in the same direction even after the direction of the electron current is reversed. This indicates that the electric current itself is not the driving mechanism for the observed motion. The authors noticed that there is a thermal gradient along the inner tube caused by inhomogeneous heating of the inner tube by the electric current. The midpoint of the inner tube is the hottest point where the temperature can reach as high as 1300 K, while the temperature near the electrodes stays at the room temperature. The authors then conjectured that the thermal gradient may have caused the outer tube to rotate and move along the inner tube. To substantiate this conjecture, they performed molecular dynamics (MD) simulations of a double walled CNT (DWCNT) in which a thermal gradient was imposed by maintaining the two ends of the inner tube at different temperatures. The simulations confirmed that the motion of the outer tube can be translation, rotation, or a mixture of both, as observed in the experiments.

There have been a number of numerical studies on thermophoretic transports of nanoparticles and water droplets through carbon nanotubes under thermal gradients. The first observation of thermophoretic force between two solid materials was presented by Schoen et al. (2006) who demonstrated controllable motions of solid gold nanoparticles inside a carbon nanotube driven by a thermal gradient along the tube. They showed that the motion of these nanoparticles is assisted by breathing vibrations of the CNT that tend to release the gold–carbon contact points (Schoen et al., 2007). Zambrano et al. (2009b) and Shiomi and Maruyama (2009) demonstrated transport of a water cluster inside a single-walled CNT (SWCNT) under a temperature gradient along the tube. Other related reports include the transports of fullerenes or short nanotubes inside (Coluci et al., 2009; Rurali and Hernandez, 2010; Somada et al., 2009; Zambrano et al., 2009a) or outside (Hou et al., 2009; Shenai et al., 2011; Tu and Hu, 2005; Tu and Ou-Yang, 2004) a SWCNT driven by thermal gradients.

The existing experimental studies and MD simulations during the last few years have firmly established the general phenomenon of nanoscale thermophoretic motion. In spite of the potential importance and generality of this phenomenon for nanoscale devices, there has been surprisingly little progress in analytical models capable of quantitative descriptions of the thermophoretic driving force between two solid objects. In the present paper, we develop an analytical model for the thermophoretic force that drives a short outer tube along an inner tube under a temperature gradient. Meanwhile, we will use the model to reveal the physical origin of a newly discovered edge force induced by atomic thermal vibration. The model will be validated through comparison with results from MD simulations.

2. Analytical model

2.1. Model description

Consider a DWCNT system consisting of a short outer tube and a long inner tube under a temperature gradient, as illustrated in Fig. 1. Previous experiments and MD simulations have shown that the outer tube will slide along the inner



Fig. 1. Schematic of a carbon nanotube thermophoretic nanoactuator composed of a long inner nanotube with length *L* and a short outer tube with length *l*. A temperature gradient is imposed on the inner tube by equilibrating atoms near its two ends at different temperatures. The thermophoretic force that drives the motion of the outer tube can be attributed to the fact that atoms with larger vibration amplitudes (due to higher temperature or lower confinement) are farther away from equilibrium, hence having higher van der Waals energy, compared to those with lower vibration amplitudes (due to lower temperature or higher confinement).

tube in the direction of the thermal gradient (Barreiro et al., 2008; Guo et al., 2011; Longhurst and Quirke, 2007; Schoen et al., 2006; Shenai et al., 2011; Zhao et al., 2010). The driving force for such thermophoretic motion can be attributed to the fact that atoms at higher temperature vibrate with larger amplitudes and are on average farther away from their equilibrium positions. Therefore, the outer tube will have higher van der Waals interaction energy with the inner tube when it is located closer to the hotter end (Fig. 1).

The present study is aimed to provide a first analytical model of thermophoretic and thermally induced forces between two solid bodies. The theory of lattice dynamics will be utilized to show that there exist two distinct contributions to the thermophoretic force in such a system. The first contribution comes from the variation of van der Waals (vdW) interaction energy along the temperature gradient, which acts on all atoms of the outer tube and will be referred to as the gradient force. The second force is associated with a newly discovered edge force near the two ends of the outer tube, which acts only on the edge atoms of the outer tube and will be referred to as the unbalanced edge force. Our analysis will show that the edge force is induced by an abrupt change in the degree of atomic confinement at the contact edge: Even under the same temperature, unconfined atoms on the inner tube that lie outside the outer tube have larger vibration amplitudes due to lower confinement and are on the average farther way from their equilibrium positions compared to those confined inside the outer tube. In this sense, while the edge force exists independent of the thermal gradient (Guo et al., 2011), it can be said to have a similar physical origin as the gradient force, although the latter exists only in the presence of a temperature gradient.

In the following, we provide a detailed derivation of these forces based on the theory of lattice dynamics.

2.2. Temperature induced vdW potential energy

A complete understanding of the thermophoretic force needs an analysis of the temperature dependent vdW potential energy between coaxial nanotubes. In the absence of thermal vibrations, the vdW potential energy has a reference value when all atoms in the system are located at their equilibrium positions. In reality, thermal vibrations cause the atoms to vibrate about their equilibrium positions, raising the vdW potential energy of the system above the reference value (see Fig. 1), which will be referred to as the temperature induced vdW potential.

We found from MD simulations that the temperature induced vdW potential energy of the DWCNT under study only has a minor dependence on the tube diameter. To simplify the calculations, we shall focus our analysis on a bilayer system consisting of two parallel graphene layers at a separation distance of 0.34 nm. We further assume that atoms in one layer (layer II) are all fixed while those in the other layer (layer I) are thermally vibrating around their equilibrium positions in the original plane (here we neglect wrinkling/folding effects keeping in mind that the radial deformation of a nanotube is very small due to its strong in-plane stiffness). The vdW potential energy between the two layers is calculated by integrating interactions between all atoms in layers I and II,

$$U_{\rm vdW} = \sum_{i} \phi_{\rm v}^{i},\tag{1}$$

where ϕ_v^i denotes the vdW interactive energy between atom *i* of layer I and all atoms of layer II. The value of ϕ_v^i should primarily depend on the vertical distance of atom *i* to layer II and vary periodically in the plane of layer II. Following the method used by Zheng and Jiang (2002), we determine $\overline{\phi_v}^i(s_i)$ as the average value of ϕ_v^i over half of a hexagonal unit cell, where s_i denotes the vertical distance of atom *i* to layer II. For small deviations $\mu_i = s_i - s_0$ of s_i from the equilibrium vertical distance s_0 , $\overline{\phi_v}^i(s_i)$ can be expressed as

$$\overline{\phi}_{\mathbf{v}}^{\mathbf{i}}(\mathbf{s}_{i}) = \overline{\phi}_{\mathbf{v}}^{\mathbf{i}}(\mathbf{s}_{0}) + \frac{1}{2}k_{\mathbf{v}\mathbf{d}\mathbf{W}}\mu_{i}^{2},\tag{2}$$

where k_{vdW} is a constant to be determined and $\overline{\phi}_v^i(s_0)$ is a reference constant whose value is of no consequence to the present analysis. We set the value of $\overline{\phi}_v^i(s_0)$ to zero so that the vdW potential energy between the two layers is expressed as

$$U_{\rm vdW} = \sum_{i} \frac{1}{2} k_{\rm vdW} \mu_i^2,\tag{3}$$

The higher the temperature is, the more dispersed the distribution of μ_i , and the higher the U_{vdW} , as schematically illustrated in Fig. 1. The total vdW potential energy can be obtained by adding up contributions from all normal vibration modes. There are a total of six branches of normal modes in graphene (Perebeinos and Tersoff, 2009), four of which are inplane vibrations and the remaining two out-of-plane vibrations. Since the in-plane vibration modes induce negligible changes in the vertical distances s_i , they can be neglected in calculating the vdW potential energy. We therefore focus on contributions from the out-of-plane normal modes.

The out-of-plane normal modes in layer I can be expressed as (Sherry and Coulson, 1956)

$$\mu_{l,m}^{A} = Z^{A} \sin(2\pi\omega t + \mathbf{r}_{l,m}^{A}; \mathbf{q}), \quad \mu_{l,m}^{B} = Z^{B} \sin(2\pi\omega t + \mathbf{r}_{l,m}^{B}; \mathbf{q})$$

$$\tag{4}$$

where $\mu_{(l,m)}^A$ and $\mu_{(l,m)}^B$ are the vertical displacements, $\mathbf{r}_{(l,m)}^A$ and $\mathbf{r}_{(l,m)}^B$ the coordinates of atoms *A* and *B* of the representative cell (l, m) (l, m = -N + 1, ..., 0, ..., N) as illustrated in Fig. 2; $\mathbf{q} = \{q_l, q_m\}$ is the wavenumber vector, ω and Z^A and Z^B are the frequency and amplitudes of the out-of-plane vibration. There are $4N^2$ cells and $8N^2$ atoms in layer I.



Fig. 2. The representative cell of graphene with in-plane base vectors r_l and r_m .

The time averaged vdW potential energy associated with a single normal mode with frequency ω is

$$U_{\rm vdW}^{\rm o} = \lim_{t_0 \to \infty} \int_0^{t_0} \sum_{l,m = -N+1}^N \left[\frac{1}{2} k_{\rm vdW} (\mu_{(l,m)}^A)^2 + \frac{1}{2} k_{\rm vdW} (\mu_{(l,m)}^B)^2 \right] dt / t_0 = \frac{1}{4} k_{\rm vdW} \sum_{l,m = -N+1}^N \left[(Z^A)^2 + (Z^B)^2 \right].$$
(5)

The total vdW potential energy can be obtained by adding up contributions from all out-of-plane normal vibration modes. Each branch of out-of-plane vibration contains $4N^2$ normal modes, so that the total vdW potential energy is

$$U_{\rm vdW} = \sum_{k=1}^{8N^2} U_{\rm vdW}^{\omega_k}.$$
 (6)

The amplitudes of normal modes Z^A and Z^B can be expressed as functions of their frequencies. Although substantial fluctuations exist in the energy associated with a single normal mode (Chen and Xu, 2011), the principle of thermodynamics demands that every single normal mode should have an average kinetic energy of $k_B T/2$ at equilibrium, where k_B is Boltzmann's constant and T is temperature. It has been shown that this equipartition of energy holds approximately in systems (Tangney et al., 2006; Zhang et al., 2009) comparable to ours. The relationship between temperature and vibration amplitude is thus

$$k_{\rm B}T = \frac{1}{2} \sum_{l,m=-N+1}^{N} m_0 \omega_k^2 [(Z_k^{\rm A})^2 + (Z_k^{\rm B})^2], (k = 1, 2, \dots, 8N^2),$$
(7)

where m_0 is the atomic mass of carbon. Combining Eqs. (5) and (7) indicates that the vdW potential energy induced by a single vibration mode with frequency ω_k is

$$U_{\rm vdW}^{\omega_k} = \frac{k_{\rm B}k_{\rm vdW}T}{2m_0\omega_k^2}.$$
(8)

Substituting Eq. (8) into Eq. (6) leads to the total vdW potential energy,

$$U_{\rm vdW} = \sum_{k=1}^{8N^2} \frac{k_{\rm B} k_{\rm vdW} T}{2m_0 \omega_k^2},\tag{9}$$

where the summation runs over all $8N^2$ normal modes.

Eq. (9) can be recast in an integral form (see Appendix A)

$$U_{\rm vdW} = \frac{8N^2}{2\sigma} \left(\iint_{\sigma} \frac{k_{\rm B} k_{\rm vdW} T}{m_0 \omega^{\rm zo} (q_l, q_m)^2} dq_l dq_m + \iint_{\sigma} \frac{k_{\rm B} k_{\rm vdW} T}{m_0 \omega^{\rm za} (q_l, q_m)^2} dq_l dq_m \right). \tag{10}$$

over the first Brillouin zone σ , where ω^{za} and ω^{zo} represent the two branches of out-of-plane vibration. Assuming the number of atoms in layer II is comparable to that of layer I ($\sim 8N^2$), the vdW potential energy per atom between layer II and layer I is

$$V_{\rm vdW} = \frac{U_{\rm vdW}}{8N^2} = k_{\rm v}T,\tag{11}$$



Fig. 3. Three kinds of atoms in Layer I when it contacts layer II.

which is clearly a linear function of temperature with

$$k_{\rm v} = \frac{k_{\rm B} k_{\rm vdW}}{2m_0 \sigma} \iint_{\sigma} \left(\frac{1}{\omega^{\rm zo}(q_{\rm l}, q_{\rm m})^2} + \frac{1}{\omega^{\rm za}(q_{\rm l}, q_{\rm m})^2} \right) dq_{\rm l} dq_{\rm m}. \tag{12}$$

This expression suggests that the vdW potential energy is mainly determined by the low frequency vibration modes.

2.3. Frequencies of out-of-plane vibration

Now let us analyze the atomic frequencies of layer I when it contacts layer II, as shown in Fig. 3.

In view of different constraints from layer II, atoms in layer I can be classified into three categories: (1) those not interacting with layer II (shown in green in Fig. 2), (2) those in full contact with layer II (shown in yellow) and (3) those near the edge of layer II (shown in red). The first kind of atoms are similar to those in a monolayer graphene, for which the frequencies of the two out-of-plane vibration modes, ω^{za} and ω^{zo} , are

$$\omega_{\text{out}}^{\text{zo}} = \sqrt{\frac{\xi + \eta}{m_0}}, \quad \omega_{\text{out}}^{\text{za}} = \sqrt{\frac{\xi - \eta}{m_0}},$$
(13)

where ξ and η are functions of the wave-number vector **q** (Appendix B).

Vibration of the second kind of atoms corresponds to that of an infinite bilayer graphene for which interlayer interactions lead to an upward shift in the out-of-plane frequency (Cancado et al., 2008; Ferrari et al., 2006). In this case, the constraint of layer II on an atom of layer I can be treated as a linear spring with stiffness k_{vdW} , and the frequencies of the out-of-plane vibration modes become

$$\omega_{\rm in}^{\rm zo} = \sqrt{\frac{\xi + \eta + k_{\rm vdW}}{m_0}}, \quad \omega_{\rm in}^{\rm za} = \sqrt{\frac{\xi - \eta + k_{\rm vdW}}{m_0}}.$$
(14)

The vibration frequencies of atoms near the edge of layer II are approximated as

$$\omega_{\text{edge}}^{\text{zo}} = \sqrt{\frac{\xi + \eta + k_{\text{vdW}}/2}{m_0}}, \quad \omega_{\text{edge}}^{\text{za}} = \sqrt{\frac{\xi - \eta + k_{\text{vdW}}/2}{m_0}}.$$
(15)

Comparisons with molecular simulations will show that this approximation is accurate enough for predicting the edge effects.

Eqs. (12) to (15) allow us to express the frequencies of the out of plane vibration modes in three distinct zones of layer I as functions of the wavenumber. The results are shown in Fig. 4 for the single layer (green line), bilayer (yellow line) and near edge zones (red line) (we follow the spectroscopic convention of expressing phonon energy in units of cm⁻¹, where cm⁻¹ denotes $hc/cm \approx 0.124$ meV). The calculated frequency dispersion for a single layer graphene is in excellent agreement with experimental data (Perebeinos and Tersoff, 2009). We can see that the frequency upshift due to the confining layer is negligible in the high frequency region, but becomes substantial in the low frequency region, especially in the region near point Γ .

2.4. Edge barrier and edge force

The vdW potential energy between an atom in layer II and all atoms in layer I is mainly determined by atoms of layer I nearest to the given atom. Therefore, the vdW potential of an edge atom in layer II interacting with layer I, V_{vdW}^{edge} , can be



Fig. 4. Phonon dispersion relations of atoms in non-contact zone (green line), full-contact zone (yellow line) and transition zone (red line) in a graphene bilayer. The circles in blue are experimental values for single layer graphene (Perebeinos and Tersoff, 2009). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

calculated from Eqs. (10) and (15), while the vdW potential associated with an inner atom of layer II interacting with layer

I, V_{vdW}^{in} , can be calculated from Eqs. (10) and (14). Clearly, V_{vdW}^{edge} and V_{vdW}^{in} are different when the system temperature is above zero, which means that there is an thermally induced edge barrier that is given by

$$\Delta V_{\rm vdW} = V_{\rm vdW}^{\rm edge} - V_{\rm vdW}^{\rm in} = (k_{\rm v}^{\rm edge} - k_{\rm v}^{\rm in})T,\tag{16}$$

where k_v^{edge} and k_v^{in} are calculated from Eq. (12) with frequencies given by Eqs. (15) and (14), respectively. According to the principle of virtual work, the above edge barrier results in an edge force on layer II

$$F_{\rm edge} = \Delta V_{\rm vdW} \frac{L^{\rm II}}{A_0^{\rm II}} = (k_{\rm v}^{\rm edge} - k_{\rm v}^{\rm in}) \frac{L^{\rm II} T}{A_0^{\rm II}},\tag{17}$$

where A_0^{II} and L^{II} are the area per atom and the length of contact edge of layer II, respectively. It is found that V_{vdW}^{edge} is always larger than V_{vdW}^{in} due to the fact that atoms in the transition zone have lower frequencies than those of the full-contact zone. This indicates that (i) a potential well can be induced when a truncated layer is attached to an extended layer, and (ii) the edge force exerted on the truncated layer points toward inside the layer, which means that there is a compressive force exerted on the truncated layer by the extended layer. These results are consistent with observations from MD simulations (Guo et al., 2011).

For a DWCNT with a short outer tube and a long inner tube, the edge forces on the two tube ends would just cancel each other in the case of a uniform temperature. However, in the presence of a temperature gradient ∇T , the resultant edge force leads to the following unbalanced edge force along the direction of decreasing temperature,

$$F_{\rm UE} = (k_{\rm v}^{\rm edge} - k_{\rm v}^{\rm in}) \frac{\pi l d}{A_0} \cdot \nabla T.$$
⁽¹⁸⁾

where A_0 is the area per atom, and d and l are the diameter and length of the outer tube, respectively.

2.5. Gradient force

Besides the unbalanced edge force, the other part of the thermophoretic force is associated with the change in vdW energy along the temperature gradient. To determine the gradient force, we note that the vdW potential energy between the inner tube and a small segment of the outer tube with length ds is

$$dV_{\rm vdW} = k_{\rm v}^{\rm in} T \frac{\pi d}{A_0} ds,\tag{19}$$

where *T* is the local temperature, and k_v^{in} is given by Eqs. (12) and (14). In the presence of a temperature gradient ∇T on the inner tube, the potential energy between the short outer tube and long inner tube is,

$$V_{\rm vdw}^{\rm tubes} = \int_{x-l/2}^{x+l/2} k_{\rm v}^{\rm in}(T_1 + s\nabla T) \frac{\pi d}{A_0} ds$$
(20)

where *x* denotes the position of the center of the outer tube center and T_1 is the temperature at the left end of the inner tube. Differentiating $V_{\text{tubes}}^{\text{tubes}}$ with respect to *x* yields the gradient force F_{grad} as

$$F_{\text{grad}} = \frac{d}{dx} V_{\text{vdw}}^{\text{tubes}} = \frac{k_v^{\text{in}} \pi l d}{A_0} \cdot \nabla T.$$
(21)

2.6. Total thermophoretic force

Combining the unbalanced edge force and the gradient force gives the total thermophoretic force

$$F_{\rm T} = F_{\rm grad} + F_{\rm UE} = \frac{k_{\rm v}^{\rm edge} \pi l d}{A_0} \nabla T.$$
⁽²²⁾

Eq. (22) indicates that the thermophoretic force is linearly dependent on the temperature gradient, as well as on the length and diameter of the outer tube. Using the dispersion relation shown in Fig. 4 and the vdW constant k_{vdW} =2.7 N/m for graphene layers (calculated based on the Lennard-Jones potential used in our molecular dynamics simulations), we find k_v^{edge} = 7.29 µeV/atom/K and k_v^{in} = 5.33 µeV/atom/K from Eq. (12). The edge barrier, edge force, gradient force, and the thermophoretic force can then be predicted from the above equations.

3. Discussion

To validate our theoretical model, we have conducted a series of MD simulations, with intra-layer C–C interactions characterized by Brenner's second generation potential (Brenner et al., 2002) and long rang Van der Waals interactions by the Lennard–Jones potential with well-depth $\varepsilon = 4.7483 \times 10^{-22}$ J and equilibrium distance $\sigma = 0.3407$ nm. A time step of 1 fs is used in all simulations.

3.1. vdW potential energy

We performed MD simulations of a bi-layer graphene, each layer containing 1200 atoms. One layer is fixed and the other is maintained at temperatures from 100 K to 500 K. We also simulated an armchair DWCNT with an interlayer distance of 0.339 nm. The lengths of the inner and outer tubes of the DWCNT are both 8 nm, and the diameter of the selected inner tube of the DWCNTs ranged from 0.7 nm to 2.8 nm. During the simulations, we first equilibrated the systems at 300 K for 100 ps, and then fixed the outer tube while maintaining the inner tube at selected temperatures ranging from 100 K to 500 K.

As shown in Fig. 5, our MD results confirmed that the interlayer vdW potential energy of bilayer graphene increases linearly with temperature at a slope of $k_v^{in} = 5.6 \ \mu eV/atom/K$, in excellent agreement with the theoretically predicted value of $5.33 \mu eV/atom/K$. When graphene sheets are rolled into nanotubes, the out-of-plane vibrations become radial vibrations. Meanwhile, the finite number of atoms along the circumferential direction causes the normal (or radial) modes to deviate from those for an infinite graphene sheet, especially when the diameter is very small. Our MD results show that the curvature of the tube affects the coefficient of the vdW energy, but not its linear dependence on temperature. By fitting the calculated values of the vdW potential energy for the DWCNTs to a linear function of temperature, we obtained a series



Fig. 5. Comparison between molecular dynamics simulation results (symbols) and theoretical predictions (line) of the van der Waals energy as a function of temperature for a graphene bilayer and carbon nanotubes.



Fig. 6. The potential coefficient as a function of the diameter of the inner tube in a double walled carbon nanotube system.



Fig. 7. The predicted and simulated thermophoretic forces in a (15, 15)/(10, 10) double walled carbon nanotube as a function of temperature gradient along the inner tube.

of size-dependent coefficients k_v^{in} , as shown in Fig. 6. It is found that k_v^{in} decreases significantly with reduced tube size when the inner tube diameter is smaller than 1.2 nm. However, when the inner tube diameter is larger than 1.2 nm, the maximum difference between k_v^{in} for a DWCNT and that for a bilayer graphene is not more than 12%. This means that our assumption that the temperature induced vdW potential energy of the DWCNT only has a minor dependence on the tube diameter is not unreasonable. For very small tubes, further studies are needed to improve the accuracy of the model.

3.2. Thermophoretic force

Next we performed MD simulations of a (15, 15)/(10, 10) DWCNT thermophoretic actuator consisting of a long (L=24 nm) inner tube and a short (L=7.3 nm) outer tube. We first equilibrated the system at 300 K for 100 ps, with the inner tube fixed at both ends. While the mean temperature was kept at 300 K, a temperature gradient is then imposed along the inner tube in the range of 0–10 K/nm by heating atoms near both ends. The system is stabilized after 50 ps. The transient force fluctuates with time as reported in the literature (Schoen et al., 2006; Xu et al., 2007). Thus, we imposed a velocity of 10 m/s on the outer tube, which is sufficiently low to ensure relatively negligible contribution from friction, and calculated the thermophoretic force on the outer tube by averaging the transient force over a long time period.

To validate our theoretical model of the thermophoretic force, we separately calculated the unbalanced edge force and the gradient force. The forces exerted on two rings of atoms on each end of the outer tube are calculated and summed together as the unbalanced edge force, while the forces exerted on all other atoms of the outer tube are summed up as the gradient force. Fig. 7 shows the unbalanced edge force and the gradient force as functions of the imposed thermal gradient. It is clear that the gradient force, the unbalanced edge force and the total thermophoretic force are all linearly proportional to the temperature gradient. The forces calculated from the MD simulations are all in reasonable agreement with our theoretical predictions.



Fig. 8. Variation of potential coefficients k_v^{in} and k_v^{edge} with the effective stiffness coefficient ξ which represents the interaction between the inner tube and inserted fillings.

3.3. Further discussion

In practice, a thermophoretic actuator is likely made of a multi-walled carbon nanotube. Besides, the inner tube of a CNT actuator may contain some nanoparticles or fluids insertions. Here we briefly discuss the effect of inserted CNTs or other fillings on the thermophoretic force. Suppose the interaction between the tube atoms and the fillings can be described by an effective spring of stiffness λk_{vdW} . In this case, the frequencies of radial vibration modes of the outermost inner tube outside the outer tube can be approximately expressed as

$$\omega_{\text{out}}^{\text{zo}} = \sqrt{\frac{\xi + \eta + \lambda k_{\text{vdW}}}{m_0}}, \quad \omega_{\text{out}}^{\text{za}} = \sqrt{\frac{\xi - \eta + \lambda k_{\text{vdW}}}{m_0}}.$$
(23)

The frequencies of the outermost inner tube inside the outer tube are

$$\omega_{\rm in}^{\rm zo} = \sqrt{\frac{\xi + \eta + (\lambda + 1)k_{\rm vdW}}{m_0}}, \quad \omega_{\rm in}^{\rm za} = \sqrt{\frac{\xi - \eta + (\lambda + 1)k_{\rm vdW}}{m_0}}.$$
(24)

The frequencies in the zone near the edge of the outer tube are

$$\omega_{\text{edge}}^{\text{zo}} = \sqrt{\frac{\xi + \eta + (\lambda + 1/2)k_{\text{vdW}}}{m_0}}, \quad \omega_{\text{edge}}^{\text{za}} = \sqrt{\frac{\xi - \eta + (\lambda + 1/2)k_{\text{vdW}}}{m_0}}.$$
(25)

Fig. 8 shows that both potential coefficients k_v^{in} and k_v^{edge} would decrease with increasing effective stiffness coefficient λ . In particular, when the inner tube is a DWCNT (in this case the actuator is made of a triple walled CNT), i.e., $\lambda = 1$, we obtain $k_v^{in} = 3.92 \ \mu eV/K$ and $k_v^{edge} = 4.45 \ \mu eV/K$. Since more inner tubes have negligible constraint to the outer tube, we know that the thermophoretic force in an MWCNT actuator could be about 73% lower than that of a DWCNT actuator.

It is noted that the thermal gradient imposed in experiments and simulations is quite high, and the efficiency of such actuators seems rather low for practical applications (Barreiro et al., 2008; Hou et al., 2009; Shenai et al., 2011). Finding efficient approaches to increasing the thermophoretic force is of significant importance. Barreiro et al. (2008) proposed that selectively exciting specific phonon modes such as the breathing mode may be a solution to reduce the thermal gradient while maintaining the thermophoretic force. Our theoretical model shows why such a solution might work: Since low frequency vibrations contribute most significantly to variations in the vdW potential and play dominant roles in the thermophoretic force, exciting lower frequency modes (i.e., the E2g mode on the order of 10 cm^{-1}), such as the breathing mode which has a relatively small frequency on the order of 100 cm^{-1} , would indeed enhance the efficiency of thermophoretic actuator systems more effectively.

4. Concluding remarks

We have presented a first analytical study of thermophoretic and thermally induced edge forces between two solid bodies. An analytical model based on the theory of lattice dynamics is developed to determine the thermophoretic force in a double walled carbon nanotube system consisting of a short outer tube sliding along a long inner tube under a temperature gradient. The model shows that the thermophoretic force is linearly proportional to the temperature gradient and the contact area (i.e., a product of the diameter and length of the short tube). The model reveals that there exist two

important components of the thermophoretic force: one is a gradient force due to variations in van der Waals potential in the presence of a temperature gradient; the other component is an unbalanced edge force induced by temperature dependent edge barriers during nanoscale contact. Our analytical model gives results in good agreement with molecular dynamics simulations.

A most important outcome of the present study is the discovery of a new type of thermally induced edge force during nanoscale contact. This edge force is induced by an abrupt change in the degree of atomic confinement at any contact edge and exists independent of thermal gradient. The physical origin of the edge force can be attributed to the fact that unconfined atoms outside the contact have larger vibration amplitudes and are on the average farther way from their equilibrium positions compared to those within the contact region. The edge force and the associated edge barrier may have profound implications on nanoscale contact mechanics and nanodevices, and much effort will be required in the future to fully explore the importance of edge forces in nanomechanics.

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Appendix A.

In the first Brillouin zone, each allowable wavenumber vector (normal mode) occupies a region of constant area (Blakemore, 1985)

$$\rho = \frac{\sigma}{M} \tag{A1}$$

where σ is the area of the first Brillouin zone and *M* is the total number of normal modes.

Eq. (10) can thus be rewritten as

$$U_{\rm vdW} = \sum_{k=1}^{M} \frac{k_B k_{\rm vdW} T}{2m_0 \omega_k^2} = \int_{\sigma} \frac{k_B k_{\rm vdW} T}{2m_0 \omega^2} \rho d\sigma.$$
(A2)

Since there are two branches of out-of-plane vibration modes, ω^{zo} and ω^{za} , Eq. (A2) can be further expressed as

$$U_{\rm vdW} = \frac{\rho}{2} \int_{\sigma} \left(\frac{k_B k_{\rm vdW} T}{2m_0 (\omega^{za})^2} + \frac{k_B k_{\rm vdW} T}{2m_0 (\omega^{zo})^2} \right) d\sigma.$$
(A3)

Using the relation (Blakemore, 1985)

$$d\sigma = dq_l dq_m \tag{A4}$$

leads to

$$U_{\rm vdW} = \frac{M}{2\sigma} \left(\int_{\sigma} \frac{k_B k_{\rm vdW} T}{m_0 (\omega^{\rm za})^2} dq_l dq_m + \int_{\sigma} \frac{k_B k_{\rm vdW} T}{m_0 (\omega^{\rm zo})^2} dq_l dq_m \right). \tag{A5}$$

Appendix B

The lattice of a single layer graphene is illustrated in Fig. 3. We consider only out-of-plane vibration of the layer. We use $\mathbf{r}_{(l,m)}^{A}$ and $\mathbf{r}_{(l,m)}^{B}$ to denote the positions of two atoms *A* and *B* in a cell (*l*, *m*). The potential energy of the entire lattice can be expressed in Taylor series as

$$U = U_0 + \frac{\partial U}{\partial \mu^{\alpha}_{(l,m)}} \mu^{\alpha}_{(l,m)} + \frac{1}{2} \frac{\partial^2 U}{\partial \mu^{\alpha}_{(l,m)} \partial \mu^{\beta}_{(k,n)}} \mu^{\alpha}_{(l,m)} \mu^{\beta}_{(k,n)} + \cdots, \quad (a, b = A, B),$$
(B1)

where U_0 is the potential energy when all atoms are at their equilibrium positions, and $\mu_{l,m}^{\alpha}$ is the out-of-plane displacement of atom α . Here repeating indices imply summation as in the Einstein convention.

For convenience, the reference energy term U_0 in Eq. (B1) is set to zero. The second term in the right hand side of Eq. (B1), $\partial U/\partial \mu^{\alpha}_{d,m}\mu^{\alpha}_{d,m}$, should vanish because the Taylor series is expanded about equilibrium positions. Keeping only the

quadratic terms in the Taylor expansion, the potential energy can be written as

$$U = \frac{1}{2} \frac{\partial^2 V}{\partial \mu^{\alpha}_{(l,m)} \partial \mu^{\beta}_{(k,n)}} \mu^{\alpha}_{(k,n)} \mu^{\beta}_{(k,n)}.$$
(B2)

The equation of motion for atom α in the cell (*l*, *m*) is

$$m_0 \frac{d^2 \mu_{(l,m)}^{\alpha}}{dt^2} + Q_{(l,m)}^{\alpha} = 0, \tag{B3}$$

where $Q_{(l,m)}^{\alpha}$ is the force exerted on atom α and can be related to the atomic displacements of the system via force constants. In practice, only contributions from the displacements of the nearest neighbor atoms are taken into account in calculating $Q_{(l,m)}^{\alpha}$. Here we consider 24 nearest neighbor atoms and thus have

$$\begin{aligned} Q^{A}_{(l,m)} &= c^{1}_{1} \mu^{A}_{(l,m)} + c^{2}_{1} (\mu^{B}_{(l,m)} + \mu^{B}_{(l-1,m)} + \mu^{B}_{(l,m-1)}) + c^{3}_{1} (\mu^{A}_{(l,m-1)} + \mu^{A}_{(l-1,m)} + \mu^{A}_{(l-1,m+1)}) \\ &+ \mu^{A}_{(l+1,m-1)} + \mu^{A}_{(l+1,m)} + \mu^{A}_{(l,m+1)}) + c^{4}_{1} (\mu^{B}_{(l-2,m)} + \mu^{B}_{(l,m-2)} + \mu^{B}_{(l+1,m-2)} + \mu^{B}_{(l+2,m)}) \\ &+ \mu^{B}_{(l,m+2)} + \mu^{B}_{(l-2,m+1)} - \mu^{B}_{(l-1,m-1)} - \mu^{B}_{(l+1,m-1)} + \mu^{B}_{(l-1,m+1)}) + c^{5}_{1} (\mu^{A}_{(l-2,m+1)}) \\ &+ \mu^{A}_{(l+1,m-2)} + \mu^{A}_{(l+1,m+1)} + \mu^{A}_{(l-1,m+2)} + \mu^{A}_{(l+2,m-1)} + \mu^{A}_{(l-1,m-1)}) \end{aligned} \tag{B4}$$

$$\begin{aligned} Q^{B}_{(l,m)} &= c_{1}^{1} \mu^{B}_{(l,m)} + c_{1}^{2} (\mu^{A}_{(l,m)} + \mu^{A}_{(l-1,m)} + \mu^{A}_{(l,m-1)}) + c_{1}^{3} (\mu^{B}_{(l,m-1)} + \mu^{B}_{(l-1,m)} + \mu^{B}_{(l-1,m+1)}) \\ &+ \mu^{B}_{(l+1,m-1)} + \mu^{B}_{(l+1,m)} + \mu^{B}_{(l,m+1)}) + c_{1}^{4} (\mu^{A}_{(l-2,m)} + \mu^{A}_{(l,m-2)} + \mu^{A}_{(l+1,m-2)} + \mu^{A}_{(l+1,m-2)} + \mu^{A}_{(l+1,m-2)} + \mu^{B}_{(l-2,m+1)}) \\ &+ \mu^{B}_{(l,m+2)} + \mu^{A}_{(l-2,m+1)} - \mu^{A}_{(l-1,m-1)} - \mu^{A}_{(l+1,m-1)} + \mu^{A}_{(l-1,m+1)}) + c_{1}^{5} (\mu^{B}_{(l-2,m+1)} \\ &+ \mu^{B}_{(l+1,m-2)} + \mu^{B}_{(l+1,m+1)} + \mu^{B}_{(l-1,m+2)} + \mu^{B}_{(l+2,m-1)} + \mu^{B}_{(l-1,m-1)}) \end{aligned} \tag{B5}$$

The solution to Eq. (B3) is

$$\mu_{d,m}^{\alpha} = Z^{\alpha} \sin(2\pi\omega t + \mathbf{r}_{d,m}^{\alpha} \cdot \mathbf{q}), \tag{B6}$$

where the wave-number vector $\mathbf{q} = \{q_l, q_m\}$ is restricted to the first Brillouin zone using Born's periodic boundary conditions. Substituting Eq. (B6) into Eq. (B3) leads to the following secular equations

$$(-m_0\omega^2 + \zeta)Z^A + \zeta Z^B = 0, \ (-m_0\omega^2 + \zeta)Z^B + \overline{\zeta}Z^A = 0,$$
(B7)

where

$$\begin{split} \xi &= c_1^1 + 4c_1^3 \cos\left(\frac{a}{2}q_l\right) \cos\left(\frac{\sqrt{3}}{2}aq_m\right) + 2c_1^3 \cos\left(\frac{a}{2}q_l\right) + c_1^5 \cos\left(\frac{a}{2}q_m\right) + c_1^5 \cos(\sqrt{3}aq_m) \\ &+ c_1^5 \cos(\sqrt{3}aq_m) + 2c_1^5 \cos\left(\frac{\sqrt{3}}{2}aq_l\right) \cos\left(\frac{3}{2}aq_m\right) + 2c_1^5 \cos(aq_l) \cos(\sqrt{3}aq_m) \\ \zeta &= \left\{ c_1^2 + 2c_1^2 \cos\left(\frac{\sqrt{3}}{2}aq_m\right) \cos\left(\frac{a}{2}q_l\right) + 2c_1^4 \cos(\sqrt{3}aq_m) + 4c_1^4 \cos(aq_l) \\ &- 2c_1^4 \cos\left(\frac{3}{2}aq_l\right) \cos\left(\frac{\sqrt{3}}{2}aq_m\right) + 2c_1^4 \cos\left(\frac{a}{2}q_l\right) \cos\left(\frac{\sqrt{3}}{2}aq_m\right) \right\} \\ &+ \mathbf{i} \left\{ 2c_1^2 \cos\left(\frac{a}{2}q_l\right) \sin\left(\frac{\sqrt{3}}{2}aq_m\right) + 2c_1^4 \sin(\sqrt{3}aq_l) - 2c_1^4 \sin(\sqrt{3}aq_m) \\ &+ 2c_1^4 \cos\left(\frac{1}{2}aq_l\right) \sin\left(\frac{\sqrt{3}}{2}aq_m\right) - 2c_1^4 \cos\left(\frac{3}{2}aq_l\right) \sin\left(\frac{\sqrt{3}}{2}aq_m\right) \right\}, \end{split}$$

 $\overline{\zeta}$ is the conjugate of ζ , and c_i^j are force constants.

The existence of nontrivial solutions to Eq. (B7) requires

$$\begin{vmatrix} -m_0\omega^2 + \xi & \zeta \\ \overline{\zeta} & -m_0\omega^2 + \xi \end{vmatrix} = 0,$$
(B8)

which consequently gives the expressions for the frequencies of the two branches of the out-of-plane vibration as

$$\omega^{zo} = \sqrt{\frac{\xi + \eta}{m_0}}, \quad \omega^{za} = \sqrt{\frac{\xi - \eta}{m_0}},$$
(B9)

with $\eta = \sqrt{\zeta \overline{\zeta}}$.

Because ω^{zo} and ω^{za} are functions of the wave-number vector **q**, we can determine the values of the force constants by fitting Eq. (B9) to the existing results. Using recent experimental data taken from Wirtz and Rubio (2004), we obtained the values of force constants as $c_1^1 = -226.93(N/m)$, $c_1^2 = 93.18(N/m)$, $c_1^2 = -7.20(N/m)$, $c_1^4 = 2.85(N/m)$ and

 $c_1^5 = -1.55(N/m)$. These values are in good agreement with other existing data in the literature. For example, using ab initio calculations, Dubay and Kresse (2004) found $c_1^1 = -248.04(N/m)$, $c_1^2 = 101.10(N/m)$, $c_1^3 = -8.10(N/m)$, $c_1^4 = 6.65(N/m)$ and $c_1^5 = -1.11(N/m).$

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