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High-speed nano-bearings constructed from double-walled carbon nanotubes: Effect of flexile deformation

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Double-walled carbon nanotubes (DWCNTs) have been proposed to be the leading candidates for high-speed nanobearings owing to superlubric characteristics between adjacent nanotubes. Performance of the DWCNT bearings is closely related to intertube friction, which is influenced by many factors, and in this work, we focus on the issue of flexibility of the nanotubes. Using molecular dynamics simulation, it has been found that considerable deformation of the nanotubes can emerge in the (5, 5)/(18, 0) DWCNT bearing with a length of ~ 80 Å if the angular speed of the shaft reaches 1.3 rev/ps. Such flexile deformation results in two distinct states with differing frictional characteristics. One of the two states, the slippery rotation, represents an interim period characterized by in-phase distortions of the inner and outer tubes, while the other state, the resistant rotation, is a steady state with the inner-tube curving lags behind that of the outer tube. Such a lag leads to a considerable increase of circular deflection of the outer tube and a sharp decrease of the minimal distance between tubes, therefore preventing the inner tube from slippery rotation.

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I. INTRODUCTION

Despite unlimited technological prospects of nano-electromechanical systems, performance, wear, and frictional properties of fundamental components of nanomachinery remain largely unknown.¹ The problem becomes critical for nanomechanical devices in which dissipation mechanism plays an important role on the performance. This is especially true for carbon-nanotube-based devices, such as molecular bearings and rotators, and axial oscillators.^{2–5} Both theoretical and experimental work uncovered that double walled carbon nanotubes (DWCNTs) can be used to construct wearless bearings with ultra-low friction.^{6–10} However, bearing friction may be enhanced with the increase of the angular speed, and rotation motion of a bearing may become unstable at some critical speed.^{9,11} Therefore, performance of DWCNT bearings is closely related to the deformability of carbon nanotubes (CNTs). It has been revealed that CNTs can sustain substantial deformation with their cross sections deviating considerably from the circular shape and the bearing central axes from a straight line. This unique flexibility of CNTs has been shown to be an important factor in enhancing intertube friction.¹¹

It has been found that the intertube friction and the performance of DWCNT devices hinge on a number of factors including the effect of temperature, commensurability, defect, size, surface edges, relative velocity, and phonons of radial breathing mode.^{3,12–17} However, the effect of the nanotube flexibility has not been given sufficient attention, despite the discovery of the effect of the wavy deformation of CNTs on intertube friction.⁵ In this work, we aim to gain

insight into the effects of the flexile deformation on the frictional behavior of DWCNT bearings. It is found that even the flexile deformation may emerge at high rotational speeds, the bearing can maintain its slippery rotation provided that the shaft deformation is in phase with that of the sleeve. However, with greater deformation, the in-phase state is no longer sustainable, and the bearings will enter a more stable state with much higher friction. The new state is subject of our further investigation, and suppression of the flexile deformation will be discussed.

The rest of the paper is organized as follows. In Sec. II, simulation methods and computational details are presented. Section III describes simulation results with a detailed discussion given on the effect of flexile deformation on the energy dissipation rate. Conclusions are drawn in Sec. IV.

II. METHODOLOGY

In this work, the method of molecular dynamics (MD) is used to study the rotational characteristics of a DWCNT bearing of (5, 5)/(18, 0) with a length of ~ 80 Å. The outer tube serves as a sleeve with one ribbon of carbon atoms at both ends fixed, while the inner tube serves as a rotational shaft with atoms at both ends constrained to drive the rotation. The applied torque may lead to large strain near the ends of the shaft and even collapse of the bearing. In order to limit the rotation-induced strain, the shaft is given a constant angular acceleration of 0.01 rev/ps² until a desired angular velocity (ω) is reached. To perform the main tasks in this work, ω is kept constant at 1.3 rev/ps after an accelerating time of 130 ps to study the effect of flexile deformation (cf. Figure 1(a), black line).

The multi-body bond-order potential by Brenner^{18,19} is used to describe intratube bonding interactions of carbon

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FIG. 1. MD results of DWCNT nanobearings. (a) Variation of the rotational speed (ω , black line) and dissipated energy (ΔE , blue line); (b) variation of the minimum interatomic distance between tubes ($\Delta_{\min}$, black line) and the intertube VDW (blue line).

atoms, while intertube long-range interactions are modeled with the Lennard-Jones 6–12 potential with parameters taken from Ref. 20. A constant temperature of 300 K is set using the Berendsen method, which couples the model to an external thermal bath with desired temperature.²¹ The rotational components in the total atomic velocity are subtracted to get the thermal components for evaluation of the thermodynamic temperature.²² At each time step, the thermal velocity is scaled by a factor

$$\lambda = \left[1 + \gamma \left(\frac{T_b}{T} - 1 \right) \right]^{1/2},$$

where T_b is the reference temperature of the thermal bath, T is the instantaneous temperature, and γ is a coupling constant, which determines the strength of the coupling to the external bath. When the inner tube rotates relative to the outer tube, intertube friction will excite high-frequency, disorderly phonon modes. As temperature is controlled to be constant, the excited energy is dissipated to the external thermal bath. Dissipated energy, ΔE , can be evaluated by

$$\Delta E = \gamma \left(1 - \frac{T_b}{T} \right) \cdot E,$$

where E is the kinetic energy determined by the thermal velocity.

III. RESULTS AND DISCUSSION

With the rotation of the inner tube, the dissipated energy accumulates as shown in Figure 1(a). Defining the slope of ΔE curve as the rate of energy dissipation (Γ), one can find two distinct rotational states of the bearing with a huge difference in Γ . From 130 ps to 1500 ps, the mean value of Γ is 1.39 eV/ps (see inset of Figure 1(a)), while the value is 741.31 eV/ps between 1520 ps and 3000 ps, about 530 times larger. As Γ correlates linearly with the intertube friction when ω remains constant,¹¹ the bearing dynamics can be divided into two distinct periods, the so-called slippery and resistant states.

To probe into the huge frictional difference between the two states, we show in Figure 1(b) the minimum interatomic distance ($\Delta_{\min}$) between the inner and outer tubes as well as the intertube Van der Waals potential (VDW). It is found that $\Delta_{\min}$ is around 3 Å in the slippery period, but decreases sharply to less than 2 Å beyond 1520 ps, while the VDW increases sharply to a much higher value. Variation of $\Delta_{\min}$

can be explicitly visualized in Figures 2(a)–2(c), which shows side-view snapshots of the DWCNT bearing. It is revealed that $\Delta_{\min}$ at 1530 ps is obviously smaller than those at 1130 ps and 1500 ps. Furthermore, side shapes of the three snapshots deviate more or less from an ideal circle. At 1530 ps, accompanying with sharp decrease of $\Delta_{\min}$, the cross section is changed greatly, leading to the quick rise of Γ after 1510 ps.

Cross-sectional changes reveal one kind of flexible deformation of CNTs. The results here show that a high angular speed can induce flexible deformation of CNTs, and consequently increase the intertube friction. We choose the central part of the CNTs to deformation characterization, as it is the most flexible part with the ends of the tubes constrained. The mean-square error displacements of chosen atoms from the tube axis is calculated and is called “circle deflection,” as it indicates the deviation of atoms of the CNTs from a perfect circle. Variation of the circle deflection is displayed in Figure 2(d), uncovering the same two states of bearings in agreement with Figures 1(a) and 1(b). In the slippery state, the circle deflection of both the inner and outer tubes fluctuates with a large amplitude, showing an unstable interim

FIG. 2. Snapshots of DWCNT nanobearings viewed along the tube axis at the time of 1130 ps (a), 1500 ps (b), and 1530 ps (c). The circle deflection as a function of time is displayed in (d).

FIG. 3. Snapshots of DWCNT nanobearings viewed perpendicular to the tube axis at the time of 1500 ps (a), and 1530 ps (b, c, viewed from different angles). The axis deflection as a function of time is displayed in (d).

state, while in the resistant state, the circle deflection is higher with smaller fluctuations, and the two tubes show great separations in the circle deflection, entering a stable state in contrast with the slippery state. The difference can be visualized in Figures 2(a)–2(c), where the circle deflection

FIG. 4. MD results of 5 DWCNT nanobearings which vary in length, radius, chirality, and speed. All the 5 bearings experience two distinct states of slippery and resistant rotation. “S” and “L” mean different length of 80 Å and 104 Å, respectively.

FIG. 5. MD results of DWCNT nanobearings with a length of ~ 55 Å. (a) Rotational speed and dissipated energy; (b) minimum interatomic distance between tubes and the intertube Van der Wall potential; (c) axis deflection showing flexible deformation.

of the inner/outer tube is 0.10/0.40 Å, 0.07/0.20 Å, and 0.22/0.52 Å, respectively, with the last one higher than the former two.

High speed rotation can stimulate another kind of flexible deformation, which is illustrated in Figure 3. The initially straight tubes are found to curve to a notable extent at 1500 ps (cf. Figure 3(a)). We define the maximum value of the deflection along the axis to be “axis deflection.” Figure 3(d) shows that the axis deflection continues to rise till a large value of ~ 3 Å is reached in the slippery state, with the inner and the outer tubes in synchronization. However, the rise of the axis deflection comes to a stop after 1510 ps, with the axis deflection of the inner tube remains around a high value of 3.22 Å, and that of the outer tube relaxes to a lower value of 1.80 Å, showing a notable difference of the axis deflection between the two tubes. Relaxation of the outer-tube axis deflection is shown in Figures 3(b) and 3(c), two snapshots at 1530 ps viewed from two different angles

perpendicular to the tube axis. The two snapshots reveal a characteristic flexile deformation in the resistant state with the outer-tube curving replaced by a local depression at the middle portion of the tube. Furthermore, the two tubes in the slippery state deform in synchronization, as shown in Figure 3(a), while in the resistant state, the axis deflection of the inner tube lags behind the local depression of the outer tube, as shown in Figures 3(b) and 3(c). The deformation lag is instrumental in preventing the inner tube from entering the slippery rotation.

We have focused on a (5, 5)/(18, 0) nanobearing with a length of ~ 80 Å to investigate the unique effect of the flexile deformation on rotational performance when the speed is confined around 1.3 rev/ps. Additional MD simulations confirm our earlier discovery of the flexibility effect. Figure 4 shows MD results similar as the blue line of Figure 1(a) for 5 different DWCNT nanobearings, which vary in length, radius, chirality, commensuration, and speed. All the nanobearings are brought to a certain angular speed at a constant acceleration of 0.01 rev/ps². Similar to what has been discussed for the (5, 5)/(18, 0) nanobearing, all the 5 bearings in Figure 4 experience two distinct states of slippery and resistant rotation, and onset of the resistant rotation is attributed to the flexile deformation.

It has been demonstrated that both circle and axis deflection can amplify friction. As a result, flexile deformation should be suppressed in the design of DWCNT nanobearings, and an effective trick is to reduce the length of the CNTs. As an example, the (5, 5)/(18, 0) nanobearing keeps its slippery state unchanged at the same speed of 1.3 r/ps when shortened from ~ 80 Å to ~ 55 Å (Figure 5(a)). The sudden drop of $\Delta_{\min}$ and the sharp increase of VDW in Figure 1(b) disappear in Figure 5(b). In addition, the axis deflection reaches a large value of ~ 3 Å in Figure 3(d), while in Figure 5(c), it is much smaller than ~ 0.6 Å for the inner tube, and than ~ 0.3 Å for the outer tube.

IV. CONCLUSIONS

DWCNTs can serve as nanobearings with a high angular speed, and flexile deformation of CNTs that comes with high-speed rotation greatly affects the intertube friction. Two distinct periods are encountered successively, namely, the slippery and resistant states. In the former, the rotation is superlubric as the energy dissipation rate is minimal, while, in the latter, friction is found to be two orders higher. The slippery rotation is characterized by synchronous deformation of the inner and outer tubes. With the increase of the axial curvature, the outer tube settles into a local depression at the central part of the tube, which brings its axis deflection out of phase with that of the inner tube, leading to considerable increase in circular deflection of the outer tube. As a result, the bearing enters its resistant state, with the cross section of the outer tube deflects greatly from its original circular shape, and the minimum interatomic distance between

tubes decreases sharply from ~ 3 Å to less than 2 Å. The bearing can work in the resistant state with an angular speed as high as 1.3 rev/ps accompanied by remarkable deformation. Furthermore, the flexile deformation can be effectively suppressed by reducing the length of the CNTs, a fact that is noteworthy in designing DWCNT nanobearings.

It should be noted that further investigations are needed to locate mechanisms responsible for substantial flexile deformation. For example, despite that the (5, 5)/(18, 0) nanobearing of ~ 80 Å in length enters a new resistant rotation at the speed higher than 1.3 rev/ps, it is found that at a lower speed of 1.2 rev/ps it maintains its slippery phase. It remains an enormous task to find mechanisms leading to the flexibility-induced resistant rotation for a given DWCNT, and to understand effects of various factors such as commensuration, defect and aspect ratio of CNTs.

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