The Intrinsic Frictional Property of Carbon Nanotubes

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Abstract. This paper aims to provide an understanding of the intrinsic frictional behaviour of CNTs under contact sliding by eliminating the possible effects of CNT rolling and slipping. Two critical steps towards the mechanism exploration were carried out: (1) the development of a new deposition method for CNT film fabrication, which allows the manufacture of densely packed, highly entangled CNT films to be firmly bonded on solid substrates for contact sliding testing; and (2) the theoretical understanding of the frictional behaviour of CNTs using the molecular dynamics analysis. The investigation clarified the controversial arguments in the literature and concluded that CNT films can be used as a superior solid lubricant with an ultra-low coefficient of friction of around 0.01.

Introduction

Investigations into the tribological behaviour of carbon nanotube (CNT) reinforced composites have led to controversial outcomes. Some studies found that the addition of CNTs to a polymer matrix can reduce the friction coefficient and wear rate of the CNT-composite [1-4], but some others reported that the use of CNTs does not improve the composite's tribological performance [5,6]. This poses an interesting question: What are the true tribological properties of CNTs?

Research on vertically aligned CNT films [7-13] seems to have produced disappointing results, showing a very high coefficient of friction, greater than 1 sometimes. Nevertheless, it was considered that these results do not really reflect the true frictional behaviour of CNTs against their sliding counterparts because the bending and local buckling of the CNTs could have substantially influenced the force variation in the sliding direction in tests. A few studies examined the friction coefficient of transversely distributed CNT films manufactured by depositing CNTs in solvent onto a quartz disk. The measured friction coefficient on such CNT films varied from 0.04 [7] to 0.09 [9], almost an order of magnitude lower than that of the vertically aligned CNT films. However, it was pointed out that the lower friction could be due to the rolling of CNTs during contact sliding, because the CNTs in the films made by the above deposition method were loosely stacked and they could roll or slip under lateral sliding forces. As a result, these measurements do not clarify the question about the true frictional property of CNTs.

This paper aims to investigate the frictional behaviour of CNTs under contact sliding without CNT rolling/slipping. Experimentally, thin films made of densely packed, highly entangled CNTs will be firmly bonded on solid glass substrates to allow high contact pressure friction test to proceed. Theoretically, molecular dynamics analysis will be carried out to explore the deformation of CNTs under contact sliding and to understand the mechanism of friction coefficient variation.

Experiment

The CNT films for tribology testing, as shown in Fig. 1, were formed on resin-on-glass substrates using multi-walled carbon nanotubes of about 15 nm in diameter and about 5 μ m in length, prepared by the chemical vapor deposition method. The resin layer provided a strong bonding with both the CNTs and the glass substrate such that CNT rolling and slipping in friction experiment were mostly eliminated.

The friction tests were performed on a micro-tribometer (CETR) under dry condition at room temperature. A conical diamond tip (tip radius = $\sim 84 \ \mu m$) was used to slide over the CNT film at the track diameter of 12 mm with the CNT film disk rotating at the speed of 0.1 rpm. Two normal loads, 1 and 10 g, were applied, respectively. The friction coefficient was calculated from the ratio of the recorded tangential force to the applied normal load. The morphologies of CNT films before and after the testing were examined on an FEGSEM6000 SEM operating at the voltage of 15kV. The SEM specimens were coated with a chromium thin film of 2 nm in thickness.



Fig. 1 An as-prepared CNT film, showing densely packed, mechanically entangled, long CNTs.

Molecular Dynamics Modelling

For computational efficiency, in the molecular dynamics analysis, only single-walled nanotubes were considered. To simulate the possible CNT orientation effect on the friction coefficient, several CNT orientation configurations relative to the diamond tip sliding direction were investigated, as shown in Fig. 2.



Fig. 2 MD models. Configuration (a): sliding perpendicular to CNT longitudinal axis, Configuration (b): sliding along CNT axis direction, Configuration (c): sliding direction in 45° with CNT axis.

CNT bundles consisting of twenty (17,0) zigzag single-walled CNTs of about 150 Å in length were arranged horizontally in rows in a closely packed arrangement as shown in Fig. 1. CNTs on the bottom row were fixed. A hemi sphere diamond tool of about 25 Å in radius was placed 3Å above the centre of a CNT on the top row, first column. The tool was moved in steps of 0.001 Å first vertically by 5Å and then laterally along the stack of CNTs. During sliding both the lateral forces and the normal forces were monitored. The lateral forces are positive when they are in the direction of sliding and negative when in the opposite direction. The sliding was carried out at different normal loads by moving the diamond tool down to 10, 15, 17.5, and 20 Å.

The inter-atomic interactions were described by a three-body Tersoff-Brenner potential which allows the formation of chemical bonds with appropriate atomic rehybridization. The non-bonded interactions between the diamond tool and the CNTs were modeled with the Lennard-Jones potential. These potentials had been used to simulate various deformation processes of carbon nanotubes [14-16].

Results and Discussion

Experimental Observation. Fig. 3 shows the variation of friction coefficient (μ) with sliding time at the normal loads (F) of 1 g and 10 g. It can be seen that μ fluctuates with its average value varying from 0.008 (F = 1 g) to 0.012 (F = 10 g). Compared with the traditional carbon materials such as graphite ($\mu = 0.1 \sim 0.3$), diamond-like carbon ($\mu = 0.05 \sim 0.15$) and PTFE ($\mu = 0.03 \sim 0.1$; one of the best lubricants), we can see that the CNT film can be regarded as a superior solid lubricant with an extremely low coefficient of friction, indicating that CNTs have a great application potential in fields with an ultra-low friction requirement. The CNT film morphology after a sliding test, Fig. 4, shows a smooth and shining surface track and no broken CNTs were found. Similar to other materials under scratching or indentation [17,18], there is a pile-up of CNTs at the track edge and the whole area of the sliding track is fully covered by carbon nanotubes, indicating that the networked CNTs in the film behave like a 'continuous material' under contact deformation. No trace of nanotube rolling was identified, demonstrating that the frictional behaviour recorded was mainly the result of sliding at the interface between the CNT film and the diamond tip. The extremely low friction coefficient observed here is a reflection of the intrinsic property of CNTs.



Fig. 3 Measured friction coefficient (μ)



Fig. 4 Sliding track on a CNT film (F = 1 g)

Theoretical Findings. The normal loads used for study were in the range from 5 nN to 30 nN. When the diamond tip slides on the nanotube compact following Configuration (a) of Fig. 2, the spinning motion of CNTs is most obvious. Under a higher load, 20.2 nN for example, more CNTs would be deformed in the depth direction, as shown in Fig. 5. Because of the discontinuous changes of the tip-CNT contacts, the forces oscillate and thus the coefficient of friction fluctuates. This is in agreement with the experimental observations described in the previous section. It should be noted that the deformation pattern varies with the relative sliding direction of the diamond tip to the CNT orientation (see configurations in Fig. 2). In relation to this, the average coefficient of friction (μ) along different directions also varies from 0.01 to 0.06, reaching its maximum when sliding under Configuration (a) (Fig. 2a) and its minimum when sliding under Configuration (c) (Fig. 2c). These coefficient values are greater than the experimentally measured ones. This is understandable, because the MD simulation was done in vacuum, but the experiment was in open air where surface contamination can reduce the strength of the tip-CNT interaction and in turn reduce the friction.



Fig. 2).



Fig. 5 CNT Deformation (Configuration (a) in Fig. 6 An example of sliding force variations (Configuration (a) in Fig. 2).

Conclusions

This paper has studied the frictional property of CNTs both experimentally and theoretically. The two approaches have led to the same conclusion that CNTs have a friction coefficient, around 0.01, in dry, contact sliding with diamond. Thus CNTs can be regarded as a superior solid lubricant with an ultra-low friction coefficient. In the investigation, CNT rolling and slipping have been minimized. It is reasonable to consider that the frictional property observed is intrinsic.

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