On the Sensitivity of Nanogripper-Carbon Nanotube Friction to Contact Area

Elnaz Haddadi
Department of Mechanical Engineering, Isfahan University of Technology, Isfahan, 8415683111, Iran

Hadi Ghattan Kashani* and Masoud Shariat panahi
School of Mechanical Engineering, Faculty of Engineering, University of Tehran, Tehran, 143955961, Iran

Hasan Nahvi
Department of Mechanical Engineering, Isfahan University of Technology, Isfahan, 8415683111, Iran

(Received 29 March 2017; Accepted 24 June 2017; Published 5 August 2017)

Despite the large volume of research dedicated to the structure and functioning of nano- electromechanical systems, few researchers have addressed the practical problems involved in their manufacture and manipulation. This paper investigates the friction phenomenon in Carbon Nanotubes (CNTs) being grasped/manipulated by a nanogripper. Molecular Dynamics (MD) simulations are employed to model the combination of friction and molecular adhesion that governs the mechanical behavior of a CNT when subjected to various loads from the gripper. It is shown that for a certain gripping force, friction between the CNT and the gripper is nonlinearly proportional to the contact area up to a certain value, and remains unchanged afterwards. This is contrary to the common belief that any amount of friction force required for detaching/relocating of CNTs could be achieved by increasing the gripping force. The implications of this finding could affect the way nanogrippers are designed for the construction/manipulation of nanoparticles. [DOI: 10.1380/ejssnt.2017.81]

Keywords: Carbon Nanotubes; Nanogrippers; Molecular Dynamics; Friction; Molecular adhesion; Contact area

I. INTRODUCTION

An extensive volume of research has been dedicated to the design and development of carbon nanotube-based electromechanical devices in nanoscale [1-8].

CNTs are commonly manipulated using silicon or other types of nanogrippers. Nanogrippers are devices that are used to manipulate particles with at least one dimension in the order of 100 nm or smaller [9]. The use of nanogrippers would allow the reliable grasping, relocating and positioning of CNTs. A typical nanogripper is shown in Fig. 1.

The grasping performance of a nanogripper is directly affected by the pressure exerted to the tube and the friction between the tube and the gripper end-effector.

Reported tribological experiments have suffered from the lack of direct observation of what takes place at the sliding interface. Although such techniques as AFM, SFA, QCM have recognized many friction phenomena in nanoscale, there are many unanswered questions regarding the interpretation of their results due to the indirect or complicated characterization of contact surfaces [10]. In spite of the critical role of friction in nanodevice-nanoparticle interactions, some of its key aspects have remained unexplored. Even in some well-studied nanoscale systems such as AFM sliding on graphite and NaCl surfaces, our perception of the microscopic mechanics of friction is still incomplete [10], and experimental observations (like the dependency of friction on temperature and velocity) have been justified based on rational arguments and simplified models [11,12]. The well-understood mechanics of friction and wear in macro-systems might be different from those in micro/nanosystems. In macroscale, tribological systems experience relatively high speeds and contact stresses compared to the micro/nanoscale. Particularly, the inertial effects that are noticeable in macroscale might be negligible in micro/nanoscale [13]. Besides, Amontons and Coulomb laws that have been used for a long time to describe dry sliding friction in macro-scale are not applicable in nanoscale [14]. Surface forces such as friction, adhesion and wear are among the main concerns in the safe design of micro and nanoelectromechanical systems (MEMS/NEMS) [15]. Accordingly, many studies have focused on the nanoscale friction in various practical systems. Guerra et al. introduce a new ‘ballistic’ friction regime in the motion of Au cluster on graphite at high speed and investigates the dependency of ballistic friction on velocity [16]. Mo et al. suggests friction laws in nanoscale for dry contacts based on results from molecular dynamics simulations [17]. The friction phenomenon at nanoscale and its various mechanisms in solid-solid and solid-liquid contacts and their relation with surface stiffness have been studied extensively [18-23]. Friction has also been studied in biological nano-machines [24] and methods have been proposed to reduce frictional energy dissipation in nanocontacts [25]. Because of the popular-

FIG. 1. A typical nano-gripper.

* Corresponding author: hghattan@gmail.com
FIG. 2. Pick-and-place of the CNTs from their as-grown position to the apex of a scanning probe tip.

FIG. 3. Configuration of a CNT being grasped by the silicon tips of a nanogripper.

FIG. 4. Potential energy of the silicon nanoplate during the equilibration phase.

II. MOLECULAR DYNAMICS METHOD

Various theoretical approaches have been used to study the friction phenomenon, including such minimalistic models as the Prandl-Tomlinson (PT) model and the Frenkel-Kontorova (FK) model, MD simulations and multicontact models like the mechano-kinetic model. The PT model is remarkably simple and helps understand many aspects of nano-friction, although it conceals the actual complexity of this phenomenon [10]. The basic, one-dimensional FK model describes friction in the onset of sliding of crystalline interfaces [27]. It is unable to study the phenomenon for the highly quasi-plastic deformations of the surfaces [28]. Multicontact models are instrumental in describing mesoscopic friction and fracture. One main problem with those models is the involvement of multiple empirical parameters [10]. MD simulations are used extensively to study sliding nano-friction. It presents a unique insight into the phenomenon and provides qualitative descriptions of atomic stick-slip. However, it is limited in the simulation size and time [10].

MD simulations are adopted here due to the fine dimensions of the components involved and the atomic discontinuity of the constituting materials.

MD simulations represent controlled computational experiments in which the dynamics of all atoms is obtained by the numerical solution of Newton (or Langevin) motion equations based on suitable inter-particle interaction potentials and the corresponding inter-atomic forces. Once the initial positions and velocities of the particles are specified, the classical differential equations of motion are numerically integrated [10]. The MD approach is widely used to model materials in nanoscale, as it provides an exact explanation of the interaction between phases in atomic scale. All MD simulations presented here are performed by using the large-scale atomic molecular massively parallel simulator (LAMMPS) [29].

MD simulations are used to study friction in nanoscale and its relation with contact area in nanoparticle manipulation using nanogrippers. Here an armchair (5,5) and a zigzag (9,0) SWCNT represent specimens and 4 nm by 5 nm silicon nanoplates with various thicknesses represent the end-effector of the nanogripper.

The manipulation modeled here is the pick and place of vertically aligned carbon nano-tubes from their as-grown position to the apex of a scanning probe tip (Fig. 2). Silicon plates that have a diamond cubic crystal structure with a lattice spacing of 5.43 Å are modeled in thicknesses of 1.0 to 5.0 nm to investigate the effect of contact area on friction force (Fig. 3).

The number of Carbon atoms in an armchair (5,5) and a zigzag (9,0) SWCNTs is 580 and 612, respectively. To take into account the no-bonding and no-charges conditions, the interactions between Si-C atoms are described by Leonard-Jones (LJ) potential with control parameters: $\sigma_{Si} = 4.0534$ Å, $\sigma_{C} = 3.4745$ Å, $\epsilon_{Si} = 0.0017354$ Å,

http://www.sssj.org/ejssnt (J-Stage: http://www.jstage.jst.go.jp/browse/ejssnt/)
FIG. 5. Snapshots of the grasping action by Si nanoplates with 2.0 nm thickness and 0.12 nm indentation depth during 5200.0 ps simulation time. (a) closing to the carbon nanotube (b) beginning the grasping (c) ending the grasping.

FIG. 6. Snapshots of the pull-out action between Si nanoplates with 2.0 nm thickness and 0.12 nm indentation depth during 8000.0 ps simulation time. (a) beginning the pull-out (b) during the pull-out (c) ending the pull-out.

$\epsilon_C = 0.0069383$ Å [30]. Also, the parameters for the interactions between CNT and silicon nanoplates are obtained by using the Lorentz-Berthelot mixing rule. The interactions among the C atoms and among the Si atoms are simulated using Brenner potential [31] and Erhart/Albe-Tersoff potential [32], respectively. Simulations are implemented in NVT ensemble under non-periodic boundary conditions in which atoms do not interact through the boundary and the locality of the boundary is set so as to envelop the atoms in that dimension, no matter how far they move. The simulation is carried out in vacuum at 300.0 K.

Each simulation includes the following three steps: equilibrating the system, grasping the CNT using the silicon nanoplates and pulling the CNT out from the nanoplates. Reasonable positioning of the atoms is achieved through equilibrating the system. Atoms of the CNT and the silicon nanoplates are equilibrated thermally to 300.0 K using a Nose-Hoover thermostat with a time step of 1.0 fs for 30.0 and 7000.0 ps, respectively.

A typical P-t curve related to the first step for one of the silicon nanoplates with a thickness of 1.0 nm is shown in Fig. 4. The curve indicates that after 2000.0 ps, the potential energy becomes steady.

Fig. 5 presents snapshots of the grasping action at a constant velocity (0.000057 nm/ps) and a time step of 0.1 fs, after the system has come to equilibrium. As indentation depth in the silicon nanoplates reaches its maximum value (0.12 nm in this study to avoid permanent damage to the silicon nanoplates and the flattening of the tube ends) they are stopped for 1000.0 ps. This process continues with a time step of 0.5 fs until the potential energy of nanoplates becomes steady. In this way, equilibration is maintained in the compressive nanoplates so that the indentation depth does not change during the simulation. This is achieved by fixing the two ends of the CNT during the second step.

In the third step, while the silicon nanoplates are fixed, the CNT is pulled out from between the nanoplates at a velocity of 0.0005 nm/ps with a time step of 0.5 fs (Fig. 6). The friction force (or the combined adhesion and friction force, to be more accurate) between the CNT and the nano-plates is determined by identifying the force required to pull out the CNT from between the nanoplates of various thicknesses based on their similarity in size. Simulation results are presented in the next section.

In order to investigate the effect of contact area on nanoscale friction, nanoplates of various thicknesses are subjected to the same indentation depth which results in various contact areas (due to the linear relation between the thickness and contact area) rather than increasing the lateral force which results in an increase in the indentation depth and the contact area.

Schematic explanation of the indentation depth and thickness are presented in Fig. 7.
FIG. 7. Schematic explanation of the indentation depth of Si nanoplate and thickness in which “T” is thickness of the Si nanoplate (defined parallel to the pulling direction) and “D” is the indentation depth achieved through averaging the indentation depths of the atoms located in the red region.

Fig. 8. Friction force as a function of time for a (5,5) CNT and various thicknesses of nanoplate a) 1.0 nm, b) 2.0 nm, c) 3.0 nm, d) 4.0 nm, e) 5.0 nm. Red lines represent mean value of the friction force.

III. RESULTS AND DISCUSSION

Fig. 8 and Fig. 9 show the variations of the friction force throughout the pull-out action for various thicknesses of the silicon nanoplates for an armchair (5,5) and a zigzag (9,0) SWCNTs, respectively, where P1 and P2 indicate the beginning and the end of the pull-out, respectively. The maximum force obtained during the pull-out action is presented in Tables I and II.

Fig. 10 presents friction force as a function of contact area during the manipulation of a CNT. Simulation results presented in Table I and Table II and Fig. 10 clearly show that the friction has a nonlinear relation with the contact area and has an upper limiting value that is not surpassed with the increase of contact area at a constant indentation depth, a point which has not been reported in previous researches that have suggested either a linear relation [33-36] or a nonlinear relation [37] between friction force and contact area.

In this study the interaction between silicon nanoplates and CNT is described by Lennard-Jones (LJ) 12-6 function; and the extent of the interactions is defined by the cutoff distance (10.0 Å according to [30]). Also, the interactions between Si-C atoms are only considered inside the cutoff distance (10.0 Å according to [30]).

Before pulling out the CNT from between nanoplates,

TABLE I. Values of friction force from various thicknesses of the gripper tip manipulating a (5,5) CNT.

<table>
<thead>
<tr>
<th>Thickness of the nanogripper tip (nm)</th>
<th>Friction force (nN)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1.72</td>
</tr>
<tr>
<td>1.5</td>
<td>1.82</td>
</tr>
<tr>
<td>2</td>
<td>1.74</td>
</tr>
<tr>
<td>2.5</td>
<td>1.9</td>
</tr>
<tr>
<td>3</td>
<td>1.7</td>
</tr>
<tr>
<td>3.5</td>
<td>1.52</td>
</tr>
<tr>
<td>4</td>
<td>1.56</td>
</tr>
<tr>
<td>4.5</td>
<td>1.46</td>
</tr>
<tr>
<td>5</td>
<td>1.58</td>
</tr>
</tbody>
</table>

84 http://www.sssj.org/ejssnt (J-Stage: http://www.jstage.jst.go.jp/browse/ejssnt/)

Haddadi, et al.
FIG. 10. Friction force as a function of thickness for a) (5,5) CNT, b) (9,0) CNT.

TABLE II. Values of friction force from various thicknesses of the gripper tip manipulating a (9,0) CNT.

<table>
<thead>
<tr>
<th>Thickness of the nanogripper tip (nm)</th>
<th>Friction force (nN)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1.73</td>
</tr>
<tr>
<td>1.5</td>
<td>1.69</td>
</tr>
<tr>
<td>2</td>
<td>2.01</td>
</tr>
<tr>
<td>2.5</td>
<td>1.51</td>
</tr>
<tr>
<td>3</td>
<td>1.62</td>
</tr>
<tr>
<td>3.5</td>
<td>1.44</td>
</tr>
<tr>
<td>4</td>
<td>1.55</td>
</tr>
<tr>
<td>4.5</td>
<td>1.33</td>
</tr>
<tr>
<td>5</td>
<td>1.66</td>
</tr>
</tbody>
</table>

The energy of the system is minimum due to its symmetry in various directions (Fig. 10). As the CNT is pulled out, the energy of the system increases due to the lack of the equilibrium, and subsequently the required force to move the CNT increases. As long as the atoms of the contact area display a local symmetry in the cutoff domain, friction does not increase significantly. As the thickness of the nanoplates increases, the distance between the edges of the nanoplate and end of the CNT diminishes, which leads to a wider region with higher friction force due to the earlier loss of the local symmetry in the cutoff domain. As the pulling continues, the value of the friction changes with the number of atoms with local asymmetry in the cutoff domain. As CNT is completely pulled out from between the nanoplates, the adhesion and friction force are gradually eliminated.

The existence of a limiting value for the friction force is justified by the observation that the interaction between atoms is limited to the cutoff domain, and even with increase in nanoplate’s thickness only the finite number of atoms with local asymmetry affect the friction.

Moreover, the friction force oscillates at the beginning of the pull-out, and its value depends on the amount of adhesion between the silicon and carbon atoms in the contact area, which decreases significantly at temperatures over 0K (300.0 K in our case) due to thermal fluctuations. It is also observed that as the lateral force increases, the indentation depth in nanoplates and hence the contact area between the CNT and nanoplate increases, and so do the force between contacting atoms and the friction force, though an upper limiting value for the friction force will continue to exist and will remain unchanged even when the nanoplate’s thickness and the nanotube’s length (and hence the contact area) are increased.

Although the above results are based on simulations involving limited number of atoms, there are no reasons to believe that they could not be extended to include similar cases involving a small contact area (such as the friction between nanoparticles and large surfaces or linear collision of plates), lack of irreversible deformations and roughness in surfaces as a result of collision pressure, as well as lack of chemical bonding between atoms at working temperatures.

The rationale behind this generalization is that in similar cases with undersized contact areas and no irreversible deformations leading to energy consumption (such as manipulation of nanotubes and nanorods) only the limited number of locally asymmetrical atoms would contribute to the generation of friction forces; and since the number of these atoms would not change with an increase in the contact area, the friction force would have an upper limiting value.

IV. CONCLUSION

The correlation between friction force and contact area throughout the grasping of a single-walled carbon nanotube by a silicon nanogripper was studied using molecular dynamics simulations. The results suggest a nonlinear correlation between the friction force and the contact area and indicate an upper limiting value for the friction force due to the fact that only the asymmetric atoms (whose number would not change with the change of contact area) contribute to the generation of friction forces. This is somewhat inconsistent with previous findings that mostly suggest a linear relation between friction force and contact area and no bounds on the former.

The coherence of the above findings indicate the possibility of extending them to other, similar situations where, due to the presence of a limited number of locally asymmetric atoms, at least one of the nanoscale contacting surfaces remains fairly smooth with no chemical bonds at the end of the lateral force application at room temperature.
ACKNOWLEDGMENTS

The authors gratefully acknowledge the Sheikh Bahaei National High Performance Computing Center (SBNH-PCC) for providing computing facilities and time. SBNH-PCC is supported by scientific and technological department of presidential office and Isfahan University of Technology (IUT). The authors would also like to thank Axel Kohlmeyer of the Institute for Computational Molecular Science, Temple University, for his valuable help and insight.