Journal of
Computational and Theoretical Nanoscience
Vol. 4, 1–4, 2007

Toroidal Carbon Nanotube as Molecular Motor

Antônio Maia de Jesus Chaves Neto* and Jordan Del Nero

Departamento de Física, Universidade Federal do Pará (UFPA), 66.075-110 Belém, PA, Brazil

In this work we propose a system that avoids the open extremities of external nanotube (NT) using a device with an external nanotube has the form of a closed ring and the internal nanotube (as a probe) in a form as semi-closed nanotube. The system consists of a rigid and static closed ring nanotube and the internal probe allowing relaxation between them (internal and external NT). The probe has asymmetric form and results in a system which presents movement by van der Waals (vdW) interactions. The simulations were made by well-known classical molecular dynamics with standard parameterizations. We calculated thermodynamics properties of these devices as molar specific heat (8.985 kcal/(mol K)) and temporary entropy variation. Properties as probe speed for this system was obtained, molecular motor efficiency versus time. In our calculations this system has 2983 carbon atoms with up to almost 7 ps of simulation. We also propose that the probe when moving (by conservation of angular moment) impels NCR in felt opposite to the probe movement, in similar way to the hamster running in a circular cage. These facts can be useful for the constructions of new molecular machines.

Keywords: Nano-Motor, Toroidal Nanotube, Molecular Dynamics.

1. INTRODUCTION

Molecular motors appear in nature in several forms as, for instance, in biological systems.[1] They are essential in the life of cells (for examples, cells of the muscle,[1] audition,[2] ...). They do load transport for your correct destiny. The motors of proteins always move along a lineal rail in a specific direction, which is dictated by some intrinsic property of the protein. It is important to know the operational physical process of the molecular motor. They organize the cell and the creation of new technological materials. Who first it looked at the molecular machines creation was Feynman[3] when inspired for the capacity of the live organisms contributing to minuscule machinery not just for the storage of information, but also for the manipulation and manufacture. He offered prizes and he paid them for the first page reduced 25000 times for an electric motor with maximum dimensions of 1/256 m edge of a cube.

As example of proteins molecular motors, we have the kinesin motor[1] that is member of a superfamily of motor proteins based on microtubes that generate force. This is the smallest known molecular motor. The motors kinesin are specialized enzymes that use the ATP hydrolysis to generate force and movement along your cellular rail, the microtubes. Masahide Kickawa et al.[4] showed that this motor presents two energy critical states. It was also found by Weels et al.[5] the behavior of molecular motor for the proteins myosins.

The rotation movement also appears for simple molecules. Komura et al.[6] have found molecular motor that is controlled by the light, consequently the space distribution of the molecules modified by the received light energy.

The auditory sensibility in mammals is larger than 40 dB due to mechanical amplification generated by a class of sensorial cells, the external capillary cells. The mechanics-electric transformation requested by the auditory sensation due to other cells capillary exteriors of the mammals they also accomplish mechanics-electric transformation. This electromobility increases the conformational variation of the voltage barrier and the prestin protein (Liberman et al.[2]) is another example of molecular motor.

In this work our proposal is simulate molecular motors with nanotubes. Since carbon nanotubes were discovered in 1991 for Iijima,[7,8] it has been attracting a lot of attention.

Cumings and Zettl[9] worked in a system consisting of fixed and movable carbon nanotubes, including a small nanotube inside. They opened an extremity in the external layer of the larger nanotube and they arrested a movable nanomanipulator in the layers of the interior nanotube. A high resolution electronic microscope allowed to study the properties of this nanosystem similar to the spring-mass behavior. They had ended that the resistance force against the sliding of the interior nanotube is small lost due to force of restoration of the van der Waals interaction

*Author to whom correspondence should be addressed.

RESEARCH ARTICLE

acting inside of nanotube pushing it outside. This experiment shows the possibility to create several systems nanomechanics operating besides a gigahertz. They also observed an amorphous residual carbon inside of exterior nanotube. This type of contamination seemingly doesn't have significant effect in the spring action. Therefore, in nanodevice terms, this contamination can create serious problems, and the ideal would be to stamp the structures in the external extremities.

The extremity problem open of the pointed external tube exists for Cumings and Zettl,[9] in that it consists of falling atoms in the extremity open of the molecular motor piston, harming or interrupting the movement.

Zheng and Jiang[10] built an van der Waals potential energy picture versus the diameter of the internal nanotube, showing that the van der Waals potential energy becomes constant with value of 6.42 10^{-21} J.

Legoas et al.[11] made the first molecular dynamics simulation for these molecular motors systems. They considered different types and nanotubes diameters (armchair, zigzag, chiral, and combinations) to verify the reliability of similar devices as oscillators in the gigahertz strip. Their results showed that the nanooscillators are stable when the radial difference values among the internal and external tubes are approximately 3.4 Å. They observed that these oscillations (in scale gigahertz) are possible for a temperature equal to 400 K. They used classical molecular dynamic simulations with standard force field, that includes the van der Waals potential. They considered structures containing above 6000 carbon atoms. This methodology has been proven that is effective in the study of dynamic properties of the carbon structures.

Guo et al.[12] hardly criticize the work of Legoas et al.[11] showing that energy dissipation really exists.

It is interesting to mention that the carbon atoms can form a nanotube closed-ring (NCR) structures with medium ray among 1500 to 2500 Å. The NCR diameter is much larger than the thickness (∼5 Å).

2. METHODOLOGY

In this work, we propose a theoretical system that avoids the open extremities[9] in the external tube. The external tube has NCR form, in other words, topologically without extremities and the internal tube working as a carbon nanotube probe (CNP). The complete system consists of a rigid and static NCR and a internal CNP relaxing (Fig. 1). Initially the energy was removed wall by potential energy interaction. This interaction could be obtained by strong and quick external electric field. We also verified that the asymmetric form of the probe results in van der Walls gradient potential resulting an acting force in the probe. The thermodynamic properties of these devices was performed, such as, molar specific heat and entropy variation. We also calculated the heat dissipation of CNP + NCR, the van der Waals properties pattern as centripetal force, energies, CNP speed. Our simulation was 2983 carbon atoms.

In this work zigzag nanotubes was used with 31[2952] atoms for CNP[NCR]. The diameter of probe was 2.733 Å and the NCR with vertical diameter equal to 5.864 Å and horizontal diameter equal to 7.894 Å. The NCR medium ray was 53 Å.

In the stationary part of the probe (over 4 ps) the probe speed is equal to approximately 2 km/s with small speed loss, soon the acting force in the probe will be the same in the Uniform Circular Movement. The probe centripetal force is approximately 10^{-10} N.

The NCR potential energy is generates by mechanical work accomplished by the van der Walls force.

Q is the heat amount emitted or received by the system, but the potential energy is that generates the mechanical work. By using of the first law of thermodynamic, we have $\Delta\mathrm{ETOT} = \Delta Q - \Delta W (= \Delta Q + \Delta\mathrm{EPOT})$. In other words, the interns energy variation of the system is translated in work donor[acceptor] and acceptor[donor] heat.

This system receives energy by external electric field and transforms in work and heat in the molecular motor. Our goal is to find a molecular motor's efficiency.

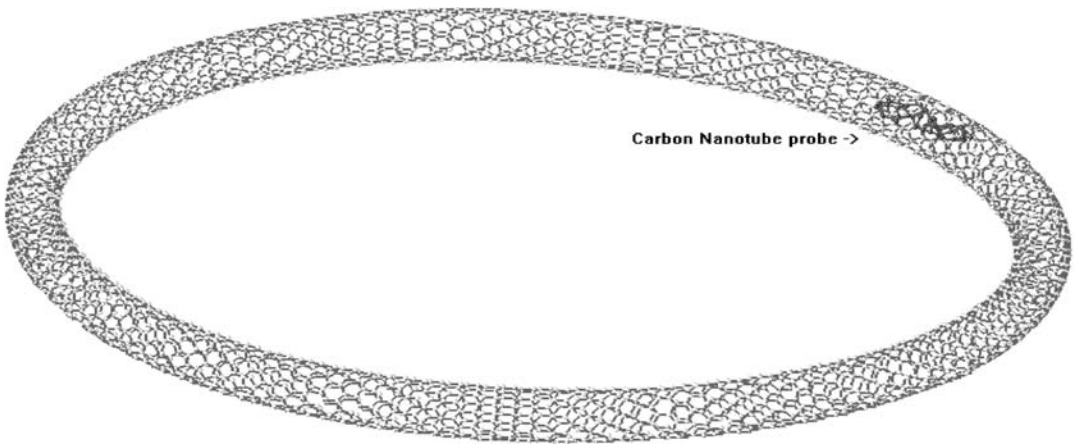

Fig. 1. Toroidal carbon nanotube (TCN) (2952 atoms) with a small carbon nanotube probe (CNP) (31 atoms), which moves as molecular motor. The simulation was made by classical molecular dynamics including standard force field.

RESEARCH ARTICLE

In this work we'll study real motors comparing with the behavior of an ideal motor, where all the processes are reversible and they don't transfer wasted energy due to friction and turbulence. We will ponder our attention to an ideal motor (motor of Carnot). This ideal motor uses the energy in the form of heat to accomplish useful work.

In this work we did the simulation at vacuo and a run time of 2000 ps with no cool time and step size equal to 0.0001 ps and the simulation was done at 500 Kelvins with the same methodology as Guo et al.[6]

3. RESULTS AND DISCUSSION

In Figure 2, we present the main properties of the molecular dynamics simulations. After 3.5 ps, the potential energy presents a small flotation owed the interaction among the atoms of NCR, being practically constant because of the great number of atoms of the NCR. The total energy varies almost directly proportional to kinetic energy similar to the spring-mass system. The kinetic energy is directly proportional the temperature. Also, it is observed that the kinetic energy possesses oscillatory form, however asymmetric, this probably happens due to fact of NCR to possess two different diameters internally (vertical and horizontal diameters), soon the probe atoms interacts in two ways with the lateral walls of NCR. Also in Figure 2 displays the kinetic and potential energy obeying the well-known behavior of highly underdamping harmonic oscillator (when the kinetic energy increases, the energy potential goes down). Figure 2 also corroborates that kinetic energy EKIN varies directly proportional to temperature. This proportionality constant is equal to EKIN/T = 8.8917 kcal/(mol K) as expected for the high temperature systems.

In Figure 2, we have that the temperature and them energy is very high in the beginning of the simulation

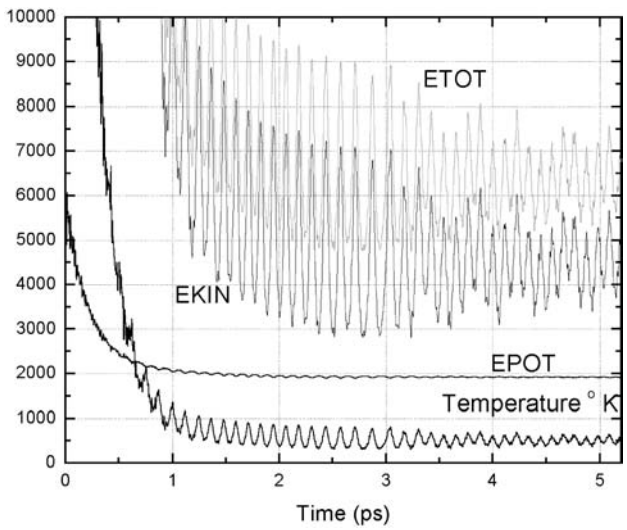

Fig. 2. Kinetic energy (EKIN), potential energy (EPOT), total energy (ETOT) (kcal/mol), and temperature (Kelvin) varying with the time of NCR + CNP.

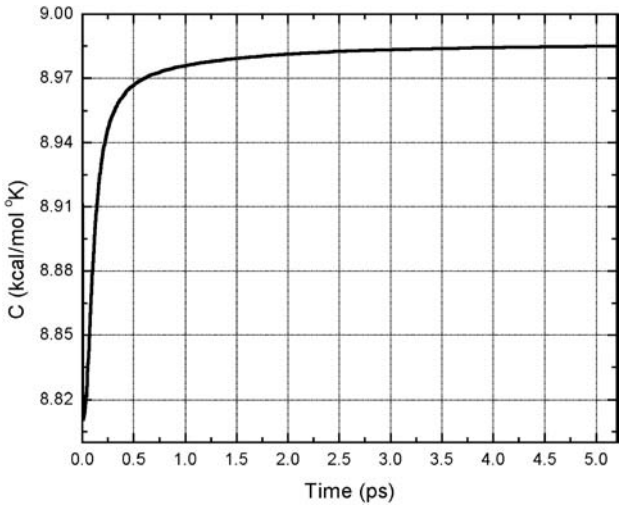

Fig. 3. Molar specific heat of molecular motor versus time.

(up to 0.2 ps) because the potential energy given by NCR walls for the probe due the intense electric field transformed in energy in heat form. After approximately 3.5 ps the system became in stationary regime, it can be said that have a change of phase of the molecular motor: phase in that the probe removes potential energy of the wall, just randomly colliding in the NCR walls and it is not moved indeed (0 < time < 3.5 ps). It transforms the kinetic energy in effective speed (after 3.5 ps) inside of NCR. This is similar with phase change of liquid state (high potential energy) to vapor state (high kinetic energy).

Figure 3 presents the molar specific heat versus time. We can see high molar specific heat in beginning (up to 0.2 ps) due the fact of molecular system to be if organizing and losing a lot of energy interns. Then the molar specific heat converges for a constant value of 8.985 kcal/(mol K).

Figure 4 presents entropy variation versus time. In the beginning (<3 ps) the entropy increases due several

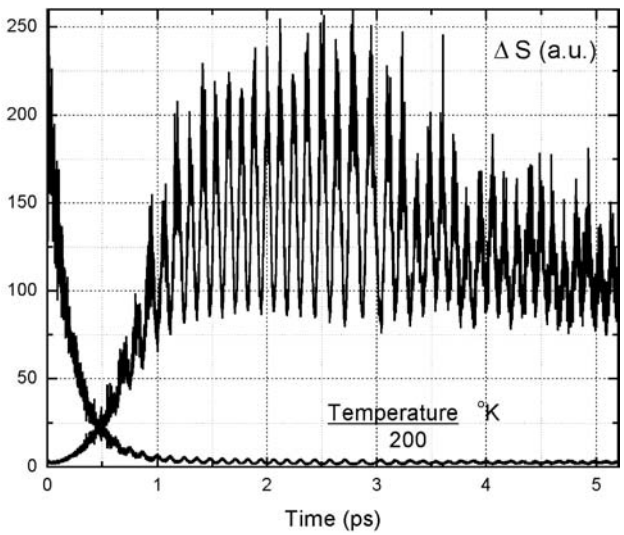

Fig. 4. Entropy variation (kcal/mol K) and temperature (K) of molecular motor versus the time.

RESEARCH ARTICLE

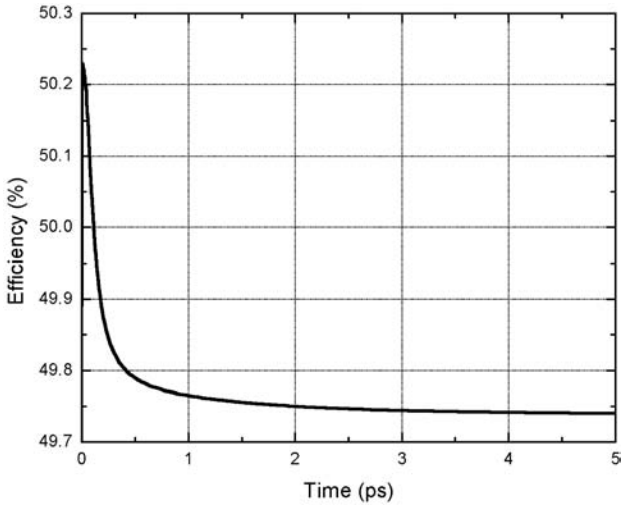

Fig. 5. Molecular motor efficiency versus time.

collisions of the probe against the NCR. After 4 ps, the entropy variation tends to be almost constant and equal to 120 a.u.

Figure 5 display the molecular motor efficiency. It is low in the beginning (<1 ps) due to loss for heat for collisions in the beginning, later it is high when the system is stabilized (>4 ps), approximately 49.74%, of the motor of Carnot.

For the probe CNP shown in the Figure 1, we have the speed, period, and frequency equal to 2 km/s, 40 ps, and 25 GHz, respectively.

For TCN + CNP system we have the kinetic energy of 4500 kcal/mol and potential energy in the stationary state same to 2000 kcal/mol using a initial temperature of 500 K (if the probe is large, the speed is small because the inertia moment[13] is large).

4. CONCLUSIONS

The kinetic energy possesses big and small variations (almost periodically) due the differences of walls interactions. Therefore the friction force will also suffer the same kind of variation due the kinetic energy to be inversely proportional to temperature.

The potential energy oscillates little by the interactions of the atoms of the NCR.

The entropy decreases when the temperature increase or when the kinetic energy decreases, meaning increase the change of information between the NCR and probe atoms and generation of phonons in toroid.

The molar specific heat has high variation in time >1.5 ps and it gets stable after 3.5 ps. The percentile rate of dissipated total energy in heat form is in order of $2 \times 10^{-5}\%$.

The dissipated potency in heat form increases in the beginning of process due to initial instability of the system probe-NCR, but after 4.5 ps the system goes to stationary state.

For symmetrical probes the system will stop because it doesn't produce potential gradient in the van der Waals forces of the NCR + probe, resulting no preferential sense.

We also propose that the probe when moving, uses the angular moment conservation, it impels NCR in felt opposite to the probe movement (similar way to the ramster running in a rotative cage). The fact of the whole NCR to rotate as a wheel in an axis it is unpublished, and it can be the base for to constructions of new molecular machines.

The calculations indicate the type of more efficient probe it would be in the asymmetric form to create a gradient of van der Waals potential. The a probe with symmetrical form has no movement due to equality of forces acting in.

Acknowledgments: We thank the UFPA-PROINT (Programa Integrado de Apoio ao Ensino, Pesquisa e Extensão) and CNPq for financial support.

References

1. F. J. Kull, E. P. Sablin, R. Lau, R. J. Fletterick, and R. D. Vale, *Nature* 380, 550 **(1996)**.
2. M. C. Liberman, J. Gao, D. Z. He, X. Wu, S. Jia, and J. Zuo, *Nature* 419, 300 **(2002)**.
3. J. Mehra, The Beat of a Different Drum, The Life and Science of Richard Feynman, Oxford University Press Inc., New York **(1994)**, p. 444.
4. M. Kickawa, E. P. Sablin, Y. Okada, H. Yajima, and R. J. Fletterick e N. Hirokawa, *Nature* 411, 439 **(2001)**.
5. A. L. Wells, A. W. Lin, L. Chen, D. Safer, S. M. Cain, T. Hasson, B. O. Carragher, R. A. Milligan, and H. L. Sweeney, *Nature* 401, 505 **(1999)**.
6. N. Komura, R. W. J. Zijistra, R. A. van Delden, N. Harada, and B. L. Feringa, *Nature* 401, 152 **(1999)**.
7. S. Iijima, *Nature* 354, 56 **(1991)**.
8. S. Iijima and T. Ichihashi, *Nature* 363, 603 **(1993)**.
9. J. Cumings and A. Zettl, *Science* 289, 602 **(2000)**.
10. Q. Zheng and Q. Jiang, *Phys. Rev. Lett.* 88, 45503-1 **(2002)**.
11. S. B. Legoas, V. R. Coluci, S. F. Braga, P. Z. Braga, P. Z. Coura, S. O. Dantas, and D. S. Galvão, *Phys. Rev. Lett.* 90, 55504-1 **(2003)**.
12. W. Guo, Y. Guo, H. Gao, Q. Zheng, and W. Zhong, *Phys. Rev. Lett.* 91, 125501-1 **(2003)**.
13. J. Liu and M. R. Spiegel, Schaum's Outline Series Mathematical Handbook of Formulas and Tables, The McGraw-Hill Companies **(1999)**.

Received: 30 April 2006. Accepted: 19 June 2006.