Journal of
Computational and Theoretical Nanoscience
Vol. 4, 1–5, 2007

Carbon Nanotubes as Gun and Molecular Motor

Jordan Del Nero and Antônio Maia de Jesus Chaves Neto*

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

In this work we propose a system as gun and molecular motor like that it uses the open extremities of external nanotube and an internal nanotube as a probe. The system consists of a rigid and static nanotube opened and the internal probe that it allows relaxation between them. The initial position of nanotubes is out of symmetry producing the probe to start the system movement due to van der Waals force acting in the probe. The simulation was made by classic molecular dynamics with standard parameterization. We calculated thermodynamic properties of these devices as molar specific heat (1.6 kcal/mol K) and temporary entropy variation (0.4 kcal/mol K). Properties as probe speed were obtained like molecular motor or gun, with the same geometry, versus time. In our calculations this system has 564 carbon atoms up to almost 50 ps of simulation. These facts can be useful for the constructions of new molecular machines.

Keywords: Molecular Motor, Nanogun, Thermodynamics, Molecular Dynamics.

1. INTRODUCTION

There is a large interest in molecular motors and a lot of knowledge can be found in living organisms. As example of protein molecular motors, we have the kinesin motor[1] that is member of a family of motor proteins based on microtubes that generate force in muscle. Masahide Kickawa et al.[2] showed that this motor presents two energy critical states. This biological molecular motor synthesis is important to development of artificial molecular machines whose progresses in artificial molecular motors are still very much in the beginning. There are two kinds of molecular motors: linear[3–6] and rotatory motors.[7] Koumura et al.[8] found molecular motor that is controlled by the light.

Cumings and Zettl[3] worked experimentally in a system consisting of fixed and movable carbon nanotubes, including a small nanotube inside. This molecular motor operated besides a gigahertz. Zheng and Jiang[4] built a van der Waals potential energy picture versus the diameter of the internal nanotube. Legoas et al.[5] made the first theoretical classical molecular dynamics simulation for these molecular motor systems. Guo et al.[6] showing that energy dissipation really exists.

In the last years, there was an explosion of papers about molecular motors trying several types in many situations, with examples the rotatory molecular[7] where were examinated the dependency of physical quantities like rotatory molecular motor, with a rotation velocity and a proton translocation rate, in the chemical reaction using the model based only in the diffusion process. Also van Delden et al. worked with motor light-driven molecular motors.[9,10] Some people studied molecular motor simulating brownian motors,[11,12] ATP molecules,[13] heart,[14] protein translocation in mitochondria,[15] processivity,[16] biochemical processes.[17]

In these researches are also calculated physical thermodinamics properties to refer to the motor like diffusion coefficients,[12] entropy and efficiency,[17,18] peclet number,[18] and others.

Already Denisov and Denisova[19] calculate the molecular motor in the sight of Coulomb interactions as well as one very interesting electromagnetism problem. They studied the background state, vibration property and deterministic transport of a chain of charged particles interacting via both the Coulomb interaction and a repulsive interaction. Derived and analyzed in detail its phonon spectrum. Also he considered the deterministic transport of a chain in a rachet potential subject to a longitudinal alternating field.

One important point of these papers is the efficiency (Eout/Ein). Miki et al.[7] carefully derived a transduction efficiency (versus the transition rate and found maximal efficiency of 53%, this result is near that found by Moon[13] (82%) values next to the Carnot cycle, Zhou et al.[18] (between 0 and 1.4%) and Igarashi et al.[20] (between 0.1% and 1%).

In this work we propose to simulate liner molecular motors with two nanotubes: one small probe nanotube inside another large nanotube in two cases: like a oscillator and a gun molecular systems.

*Author to whom correspondence should be addressed.

RESEARCH ARTICLE

2. METHODOLOGY

In this work, we propose a theoretical system with the opened extremities[4] in the external tube. The external tube has NCE form with extremities and the internal tube working as a carbon nanotube probe (CNP). The complete system consists of a rigid and static NCE and a internal CNP relaxing (Fig. 1). Initially the energy was removed wall by potential energy interaction. This interaction could be obtained by strong external electric field. We also verified that the asymmetric initial position of the probe results in van der Walls gradient potential resulting a acting force in the probe. The thermodynamic properties of these devices were performed, such as, molar specific heat and entropy variation. Also we calculated the heat dissipation of CNP+NCE, the van der Waals properties pattern as force, energies, CNP speed. Our simulation was to 560 carbon atoms.

In this work zigzag nanotubes were used with 24[540] atoms for CNP[NCE]. The diameter and length of probe were 2.457 and 6.358 Angstrons and the NCE with diameter and length equals to 6.725 and 61.976 Angstrons.

The NCE potential energy is generated by mechanical work accomplished by the Van der Waals force.

By using of the first law of thermodynamics, we have that internal energy variation of the system is translated in work donor[acceptor] and acceptor[donor] heat.

In the beginning, this system receives energy by external electric field and turns it into work and heat in the gun and molecular motor. In case of molecular motor, our goal is to find a molecular motor with maximum efficiency with the minimum of dissipated energy and heat dissipation due to the friction of inelastic collisions between the probe and NCE atoms. The molecular motor could also be used like a molecular gun with other very different characteristics.

In this work we studied theoretical motors comparing with the behavior of an ideal motor. We will ponder our attention to a ideal motor, the motor of Carnot. We did the simulation at vacuum 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 dynamic simulations to molecular motor. The potential energy always presents a small flotation owing to the interaction among the atoms of NCE, because of the great

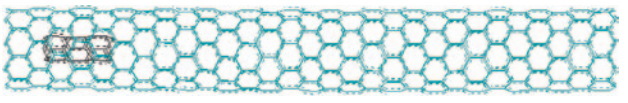

Fig. 1. Nanotube of carbon (CNE) (540 atoms) with a small carbon nanotube probe (CNP) (24 atoms), which moves as molecular gun or motor. The simulation was made by classical molecular dynamics.

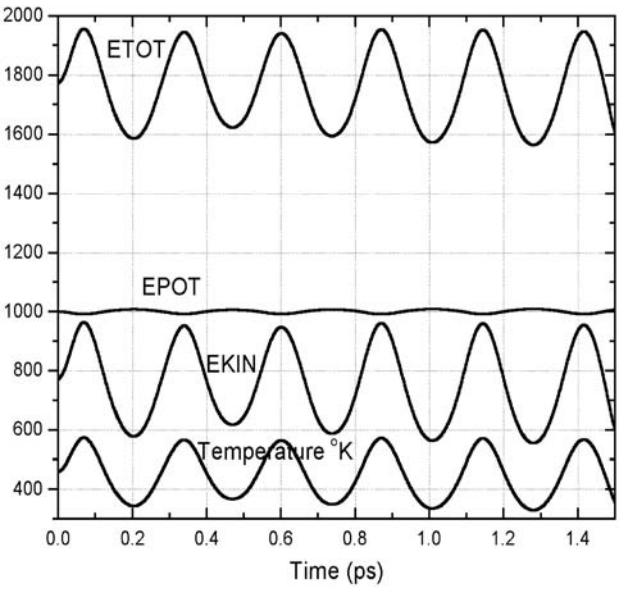

Fig. 2. Kinetic energy (EKIN), potential energy (EPOT), total energy (ETOT) (kcal/mol), and temperature (Kelvin) varying with the time of NCE+CNP of molecular motor.

number of atoms of the NCE. The total energy varies almost directly proportional to kinetic energy similar to the spring-mass system. The kinetic energy is directly proportional to the temperature. It is also observed that the kinetic energy has oscillatory form. Also in Figure 2 displays the kinetic and potential energy obeying the well-known behavior of high underdamping harmonic oscillator (when the kinetic energy increases, the energy potential goes down). Figure 2 also corroborates so that the kinetic energy EKIN varies directly proportional to the temperature. This proportionality constant is equal to EKIN/T = 1.6811 kcal/(mol K) as expected for the high temperature systems.

For the CNE+CNP molecular motor system, we have the kinetic energy of 0.8 Mcal/mol and potential energy in the stationary state same to 1.0 Mcal/mol using a initial temperature of 500 K (if the probe is large, the speed is small because the inertia moment of NCE is large). For the probe CNP shown in the Figure 1, we have the frequency equal to 4.0×10^{12} Hz. In this case, the stationary part of the probe (over 1 ps) the maximum probe speed is equal, approximately, to 0.450 km/s, soon the acting force in the probe will be the same as in the oscillator movement.

In Figure 3, we present the main properties of the molecular dynamic simulations to molecular gun. After 0.4 ps, the potential energy presents a small flotation owing to the interaction among the atoms of NCE, being practically constant because of the great number of atoms of the NCE. The total energy varies almost directly proportional to kinetic energy similar to the gaseous system. The kinetic energy is directly proportional to the temperature. It is also observed that the kinetic energy has temperature form, since the probe atoms interact in two ways

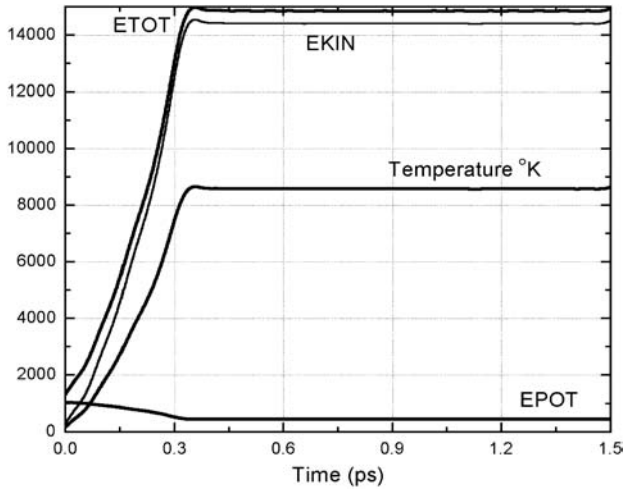

Fig. 3. Kinetic energy (EKIN), potential energy (EPOT), total energy (ETOT) (kcal/mol), and temperature (Kelvin) varying with the time of NCE + CNP of molecular gun.

with the lateral walls of NCE. Also in Figure 3 displays the kinetic and potential energy obeying the well-known behavior of gaseous expansion. Figure 3 also corroborates so that kinetic energy EKIN varies directly proportional to the temperature. This proportionality constant is equal to EKIN/T = 1.6811 kcal/(mol K) (is the same exact value of molecular motor) as expected for the high temperature systems.

In case of molecular gun the stationary part of the probe (over 0.32 ps) the probe speed after launch is equal to 4.31 km/s with huge energy lost in heat form because of this system uses, basically, a lot of molecular energy of the external NCE tube and molecular energy of the probe CNP, since the acting velocity in the probe will be the same in the Uniform Movement after launch.

In Figure 3 we have that the temperature and the kinetic energy are increasing in the beginning of the simulation

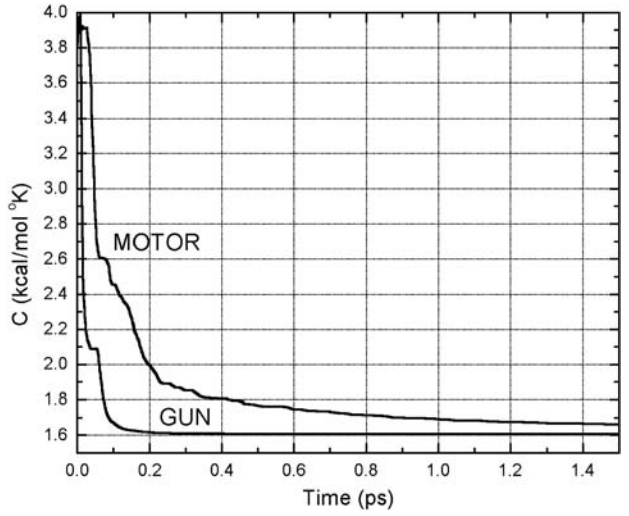

Fig. 4. Molar specific heats of molecular gun and motor versus time.

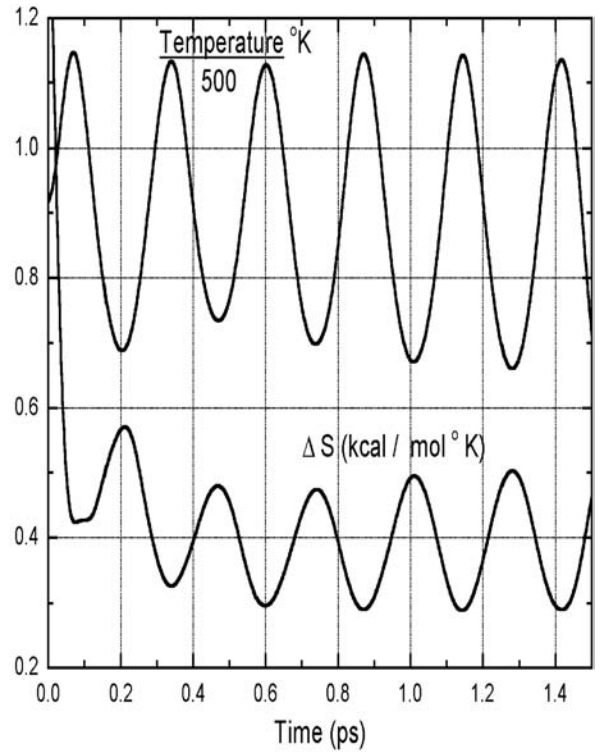

Fig. 5. Entropy variation (kcal/mol K) and temperature (K) of molecular motor versus the time.

(<0.3 ps) because of the potential energy given by NCE walls for the probe due to the intense electric field turning kinetic energy into heat form. After approximately 0.32 ps the system became a stationary regime, it can be said that has a change of phase of the molecular gun: phase in which the probe removes potential energy of the wall, the NCE walls change its form and it is not moved indeed (0 < time < 0.3 ps). It turns the potential energy into effective speed (after 0.32 ps) ejecting the probe out of NCE. This is similar with the phase change of the liquid state (high potential energy) to vapor state (high kinetic energy).

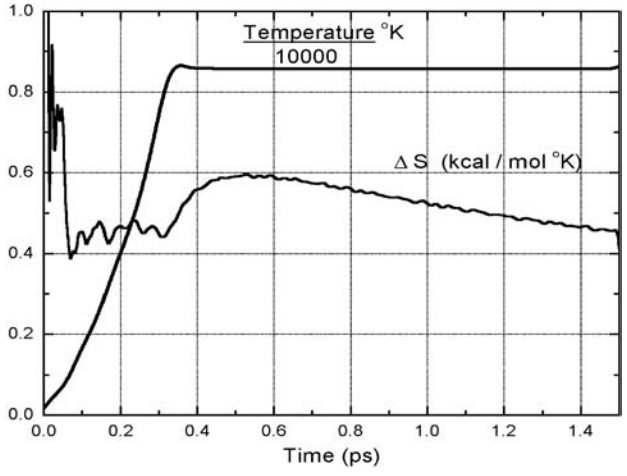

Fig. 6. Entropy variation (kcal/mol K) and temperature (K) of molecular gun versus the time.

RESEARCH ARTICLE

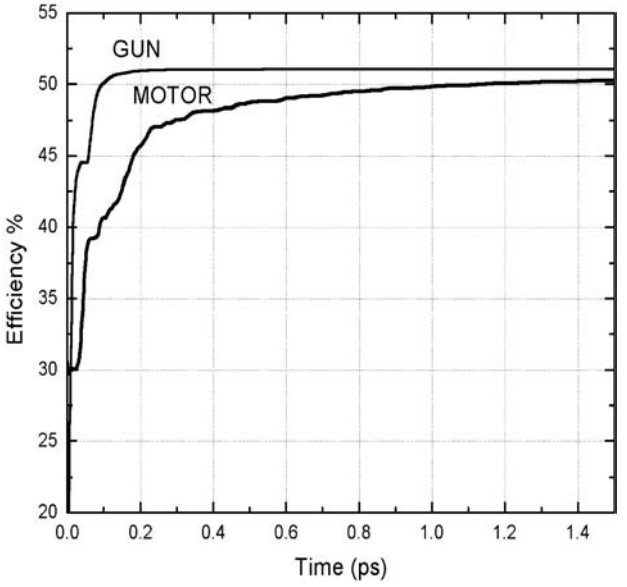

Fig. 7. Molecular motor and gun efficiencies versus time.

For the CNE + CNP system of molecular gun, for CNE + CNP system we have the kinetic energy of 14.0 Mcal/mol and potential energy in the stationary state same to 0.5 Mcal/mol using a initial temperature of 500 K (if the probe is large, the speed is smaller because the mass of NCE is large).

Figure 4 presents the molar specific heat of molecular gun and molecular motor versus time. We can see high molar specific heat in beginning (down to 0.34 ps due to the molecular system to be organizing and losing a lot of energy interns (the nanogun get stable first)). Then both the molar specific heat converges for the same constant value of 1.681 kcal/mol K.

Figure 5 presents entropy variation of molecular motor versus time. In the beginning (up to 0.1 ps) the entropy increases due to several collisions of the probe against the NCE. After 0.1 ps, the entropy variation tends to be almost constant in average value of 0.4 kcal/mol K.

Figure 6 presents entropy variation of nanogun versus time. In the beginning (up to 0.5 ps) the entropy is high repulsion of the probe by NCE and NCE great deformation's. After 0.5 ps, the entropy variation tends to decrease to the value of 0.4 kcal/mol K, asymptotically.

Figure 7 displays the molecular motor and the gun efficiency. It is low in the beginning ($<$0.32 ps) due to lost of heat by collisions in the beginning, later it is high when the system is stabilized ($>$0.32 ps), approximately 51.25%, of the order of motor of Carnot.

4. CONCLUSIONS

The kinetic energy is directly proportional to the temperature. The potential energy decreases when kinetic energy increases. The potential energy oscillates little due to the interactions of the huge number of atoms of the NCE.

The entropy decreases when the temperature increases or when the kinetic energy decreases, meaning increased of the change of information between the NCE and probe atoms and generation of phonons in the system NCP-NCE.

The molecular motor molar specific heat varies in time $>$1 ps and it becomes stable after 1 ps. The molecular gun molar specific heat varies in time $>$0.32 ps and it becomes stable after 0.32 ps. Both tends to the same value.

The dissipated potency in heat form increases in the beginning of process due to the initial instability of the system NCP-NCE, but after 1 ps the system goes to stationary state for the molecular motor. After 0.32 ps the system goes to stationary state for the molecular gun and it demands a lot of heat of NCE.

For initial symmetrical geometries (probes in the center NCE) the system does not work because it does not produce potential gradient in the van der Waals forces of the NCP + NCE, resulting no preferential sense.

The efficiency was low in the beginning due to the lost of heat by collisions in the beginning, later it is high when the system is stabilized approximately of the order of motor of Carnot and this efficiency agrees with results of Miki et al.,[7] Moon and Park.[13] The nano gun system can be stable firts, because the NCE does not interact with the distant probe.

The molar capacity heat, entropy (in average value) and efficiency of the molecular motor converge asymptotically to the results of the molecular gun in case of large times.

In the future, very well controlled molecular gun could be used to attack cancer or wax cells (it placed like oscillator motor in the direction of the cancer and after it is activated the external electric and the molecular gun shot the target). Also, the molecular gun could be used like a propulsive rocket to transport the nanorobots.

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

References

1. F. J. Kull, E. P. Sablin, R. Lau, R. J. Fletterick, and R. D. Vale, *Nature* 380, 550 **(1996)**.
2. M. Kickawa, E. P. Sablin, Y. Okada, H. Yajima, R. J. Fletterick, and N. Hirokawa, *Nature* 411, 439 **(2001)**.
3. J. Cumings and A. Zettl, *Science* 289, 602 **(2000)**.
4. Q. Zheng and Q. Jiang, *Phys. Rev. Let.* 88, 45503-1 **(2002)**.
5. S. B. Legoas, V. R. Coluci, S. F. Braga, P. Z. Braga, P. Z. Coura, S. O. Dantas, and D. S. Galvão, *Phys. Rev. Let.* 90, 55504-1 **(2003)**.
6. W. Guo, Y. Guo, H. Gao, Q. Zheng, and W. Zhong, *Phys. Rev. Lett.* 91, 125501-1 **(2003)**.
7. H. Miki, M. Sato, and M. Kohmoto, *Phys. Rev. E* 68, 61906 **(2003)**.
8. N. Koumura, R. W. J. Zijistra, R. A. van Delden, N. Harada, and B. L. Feringa, *Nature* 401, 152 **(1999)**.

9. R. A. van Delden, N. Koumura, A. Schoevaars, A. Meetsma, and B. L. Feringa, *Org. Bio. Chem.* 1, 33 **(2003)**.
10. R. A. van Delden, M. K. J. ter Wiel, H. de Jong, A. Meetsma, and B. L. Feringa, *Org. Bio. Chem.* 2, 1531 **(2004)**.
11. D. Dan, A. M. Jayannavar, and G. I. Menon, *Physica A* 318, 40 **(2003)**.
12. K. Sasaki, *J. Phys. Soc. Jpn.* 72, 2497 **(2003)**.
13. H. Y. Moon and Y. Park, *Phys. Rev. E* 67, 51918 **(2003)**.
14. P. P. de Tombe, *J. Biomech.* 36, 721 **(2003)**.
15. H. C. Loebl and C. C. Matthai, *Physica A* 342, 612 **(2004)**.
16. X. Ping, S. X. Dou, and W. Peng-Ye, *Chin. Phys.* 13, 1569 **(2004)**.
17. C. Maes and M. H. van Wieren, *J. Stat. Phys.* 112, 329 **(2003)**.
18. Y. Zhou and J. D. Bao, *Physica A* 343, 515 **(2004)**.
19. S. I. Denisov and E. S. Denisova, *Phys. Rev. B* 68, 64301 **(2003)**.
20. A. Igarashi, H. Goko, and S. Tsukamoto, *Physica A* 325, 62 **(2003)**.

Received: 11 July 2006. Accepted: 6 September 2006.