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MD Simulation of Brownian Motion of Buckminsterfullerene Trapping in Nano-Optical Tweezers

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Abstract Optical tweezers are a relatively new technique for non-invasive manipulation tool in biology and physics for studying single molecules. Brownian motion of a trapped particle poses a challenge to develop the Optical tweezers. Standard methods to analyze the optical tweezers data rely on using power spectrum of the Brownian motion of a dielectric bead trapped in the tweezers for macro scales. In this study the well-known MD code, GROMACS, is modified to find the variation of position and velocity of all atoms in the system of buckminsterfullerene solved in water. By applying the statistical methods our molecular dynamics simulations reveals the diffusion coefficient of the motion and the standard deviation of the Brownian motion. The simulation of system performs for the variety of trap constant and a model for estimation of the diffusion coefficient and the standard deviation of the Brownian motion is presented. Finally, experimental results are discussed based on the proposed model.

Keywords Optical tweezers, Brownian motion, Viscous effects, Molecular dynamics

1. Introduction

In recent years, advancement of technology from micro [1] to nanoscales [2], many theoretical phenomena have found their importance in emerging applications. One of this phenomena is the optical tweezers. Optical tweezing applies a powerful laser beam focused by lens to trap or rotate particles such as cells or nanoparticles, which are suspended in a damping medium such as water [3-4]. In biology and in physics, there has been a common interest in single molecules with sizes ranging from 1 nm to 1 μm [5].

In recent years a new microsystem has proposed for automated electro rotation measurements using laser tweezers [6]. In that reference, the optical tweezers are used as a bearing system for rotational studies for determining cytoplasmic properties. To compute this phenomenon, one should use the molecular dynamics other than common methods in macro scale bearings [7-10] such as general Reynolds equation theories [11-13]. Besides Brownian motion at short time scales, many groups currently track theoretical and experimental studies of isotropic Brownian motion in equilibrium systems. The forces and stains induced by biological molecular motors are in the range of picoNewtons (pN) [6,14]. For biological specimens, a common experimental task is the measurement of the viscoelastic properties of single biopolymer such as DNA, cell membranes, aggregated protein fibers such as actin, gels of such fibers in the cytoskeleton, and composite structures such as chromatin and chromosomes [15,16]. Nowadays the control of molecules is interest of many scientific fields [17]. The importance of numerical simulation of nano-Optical tweezers is in fact that obtaining effective diffusion in such sizes is so expensive [18]. Buckminsterfullerene or bucky-ball is a spherical fullerene molecule with the formula C_{60} can be found in small quantities in soot. It has a cage-like fused-ring structure which resembles a soccer ball, made of 20 hexagons and 12 pentagons, with the 60 carbon atoms present at each vertex of each polygon and a bond along each polygon edge [19]. The buckminsterfullerene molecule is extremely stable, enduring high temperatures and high pressures and atoms can be entrapped at the interior without reacting [20]. As the thermal radiation has its applications in macro scale [21-29] it used for micro and nano-scale for trapping [30-33]. The numerical modelling of this phenomenon is appeared in many researches [34-40]. In this paper, the MD simulations used to finding the characteristics of Brownian motion of trapped particle from its position and the amplitude of viscous force is derived from the velocity of the trapped particle.

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2. Optical Trap Dynamics

Optical tweezers tools use the forces of laser radiation pressure to trap small particles (see figure 1).

For photons the force of collision is

$$\vec{F} = -\frac{d\vec{p}_{photon}}{dt} \quad (1)$$

When the particle radius '*a*' is larger than the wavelength of the light λ there is Ray optics regime (Mie scattering $F_r = Q\frac{n_s}{c_0}P_i$) and Rayleigh scattering vice versa.

Light generates 2 types of optical forces: scattering and gradient scattering force and gradient force are separable. The dipole moment is $\vec{p} = \alpha\vec{E}$ in which Dipole polarizability is

$$\alpha = n_s^2 \frac{m^2 - 1}{m^2 + 2} \cdot a^3 \quad (2)$$

so the gradient force is

$$\vec{F} = (\vec{p}\nabla)\vec{E} + \frac{\partial \vec{p}}{\partial t} \times \vec{B} = \frac{\alpha}{2}\nabla E^2 \to F_{grad} \propto a^3 \cdot \nabla I_{inc} \quad (3)$$

where a is the particle radius and I is the incidence power. But the scattering force [34]

$$F_{scat} = \frac{n_p}{c_0}P_{scat} \propto C_{scat}I_{inc} \propto a^6\lambda^{-4} \cdot I_{inc} \quad (4)$$

is proportional to the scattering cross-section. For trap stability $F_{grad} > F_{scatt}$ requires tight focusing. (K_b=1.3806488 × 10^{-23} m^2 kg s^{-2} K^{-1} and the value AMU=1.66×10^{-27} kg so the stiffness is (1 kg.s^{-2}=1 N/m=602.2 amu/ps^{-2}). (C_{scat} is a function of medium refractive index contrast and light speed. for more information see [41]).

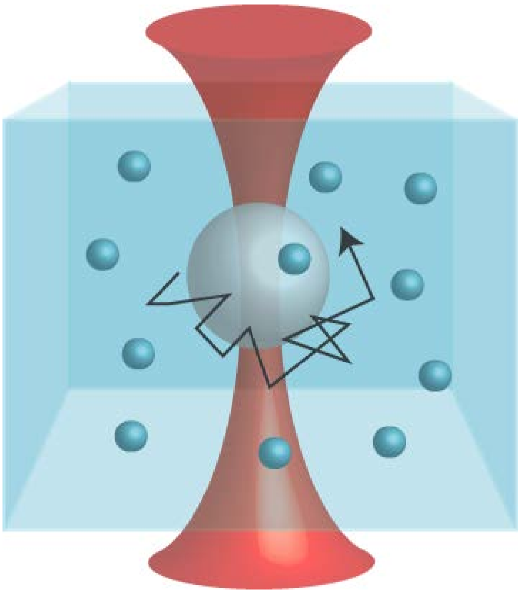

Figure 1. Schematic of optical tweetzer [5]

Equation of motion of particle in a potential well contains Newtonian force, restoring force (with spring constant κ which cause to harmonic motion), drag force (with Damping factor of $c=6\pi\eta r$ which appears in exponential decay), and Brownian motion (Time averaged effect is 0 i.e. $<F(t)F(t')>$ $= 2k_BT\gamma\delta\,(t-t')$). In Langevin equation:

$$m\ddot{x} + c\dot{x} + kx = \vec{F}_B(t) \quad (5)$$

If a known force is applied (F_B is given), and the displacement is measured, the 'stiffness' of the optical trap (Trap strength depends on light intensity, gradient $k_{trap} \approx k_{bio} \approx 0.1$pN/nm) may be determined:

$$k = \frac{6\pi\eta r v}{x} \quad (6)$$

But the Stochastic events introduce fluctuations in the particle's position.

3. Results

For molecular dynamics (MD) an appropriate force field is required that can adequately describe the potential energy for water molecules. In this study, the GROMACS version 4-6-1 is used [42]. The using of GROMACS code and its efficiency to calculate diffusion constants is common. GROMACS utilize both Einstein and Green-Kubo equations. At the initial condition of the MD simulations, trapped molecule is fixed and let the water molecules to move and soak it. The overall MD simulation with duration of 100 ps was performed. Weak coupling of the trapped molecule to a solvent bath of constant temperature (300 K) and constant pressure (1 bar) was maintained with a coupling time of 1.0 ps. The simulation was carried out at a temperature of 300° K. An integration step of 1.00 ps was used throughout all simulations. The current simulations contains 30000 water molecules in the box domain which each side equal to 10 nm.

Important specifications in the grompp input file related to context are as: the integrator is md with time difference equal to 0.001 (in MD units) with 12000000 steps. Neighbor searching algorithm is grid with 10 atoms in list and freezes the wall during the energy minimization. nose-hoover algorithm is used for coupling with τ=0.2 and reference temperature of 300 K (Gen seed = 94729). The PME is used for coulomb force with radius 1.1(in MD units) and Fourier spacing equal to 0.15 by ewald tolerance of 1×10^{-5}.

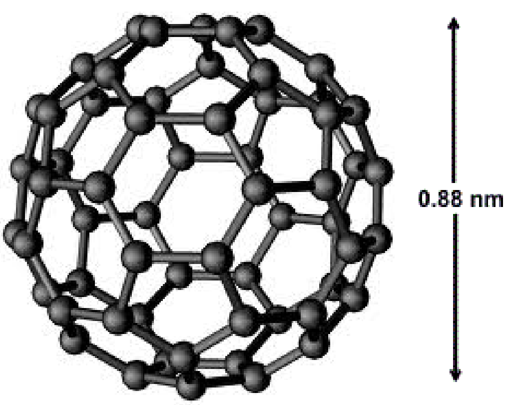

Figure 2. Schematic of buckminsterfullerene

Figure 4 shows the angular positions (θ) and the rate of the change of the angular displacement (ω) for the control case. Except the beginning of the motion, in which buckminsterfullerene is under soaking interaction with the fluid, there is not a significant change in the angular positions (θ) of our trapped buckminsterfullerene. So the angular stiffness of buckminsterfullerene in nano-Optical tweezers can be ignored for practical estimations *i.e*

$$\frac{1}{2}k\bar{x}^2 = \frac{1}{2}m\bar{v}^2 + \frac{1}{2}I\omega^2 \quad (7)$$

By taking the fast Fourier transform of the motion of the buckminsterfullerene in nano-Optical tweezers the amplitude spectrum of a measured signal is calculated. Figure 5 shows the periodogram spectrum of velocities positions for the control case. In each part, the vertical axis is the power spectral density (PSD) estimate of the sequence while the horizontal axis is the corresponding vector of frequencies which is computed in radians per sample. The power spectral density is calculated in units of power per radians per sample. Because periodogram spectrum of positions is near to Gaussian distribution, the ideal position spectrum of a bead in an optical trap can be used to determine the stiffness of the trap.

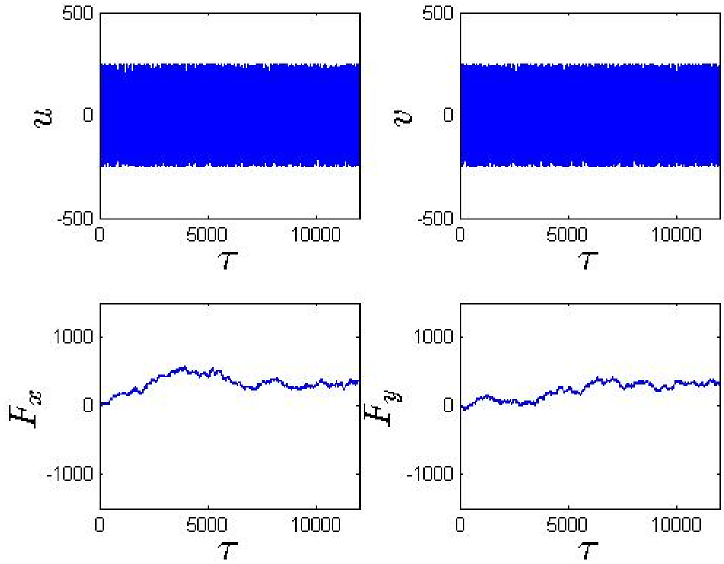

Figure 3. Velocity, and force components for k=0.01 trap stiffness

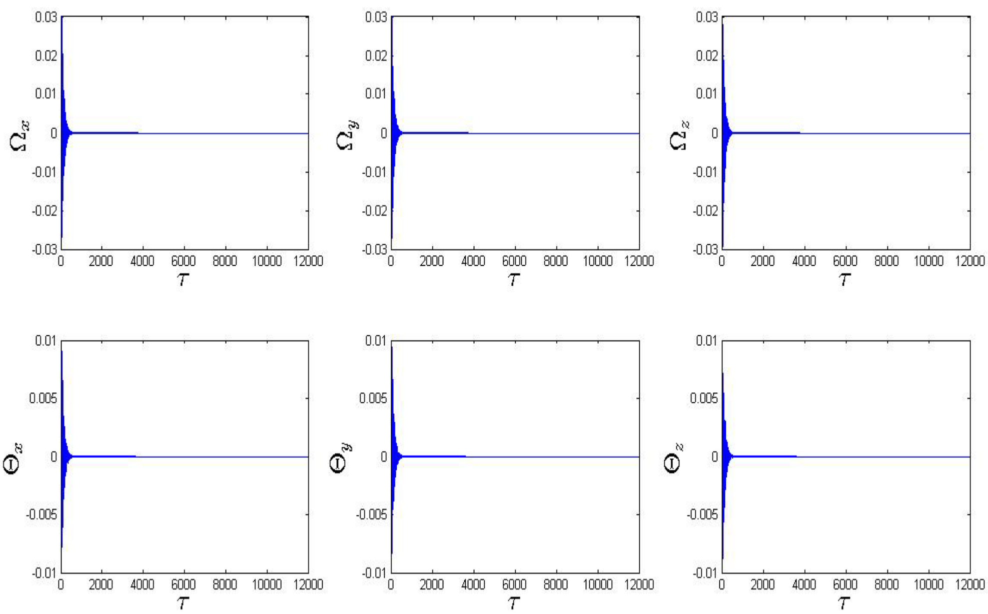

Figure 4. Angular positions and the angular velocities for the control case

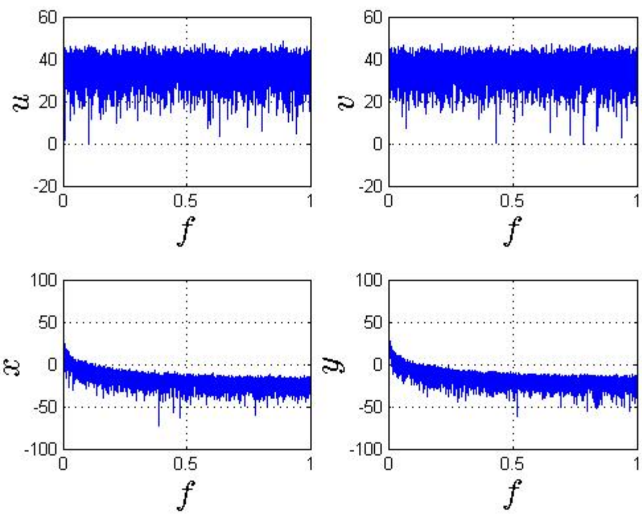

Figure 5. Periodogram spectrum of positions and velocities for the control case

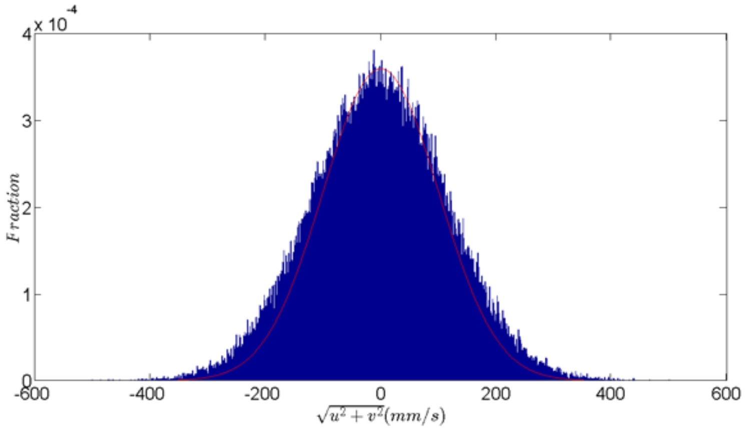

Figure 6. Fraction of buckminsterfullerene velocity magnitude over the time for k=0.1 trap stiffness

Figure 6 shows the Fraction of buckminsterfullerene velocity magnitude over the time for trap stiffness k=0.1. A normal probability density function for the one-parameter distribution is fitted on the figure by red line. The normal distribution of the velocity magnitude around the mean values of it demonstrates the stochastic characteristic of the motion. It happens because in GROMACS the Nosé–Hoover thermostat is applied in each iteration step.

The limitation applied on the motion by various trap parameters is presented in Figure 7. That figure shows the Fraction of buckminsterfullerene position over the time for high and low trap stiffness is obtained from the statistical calculations. In addition, the fraction spectrum of the position is presented for each case. Persistence and randomness which are two key characteristics of Brownian motion can see in figure 7-a.

It seems that the Brownian motion is simulated approximately isotropic. As demonstrated in figure 7-b by increase of the trap stiffness the maximum distance from the position decreased and the buckminsterfullerene is more confined to the trap center and the trap performance increased.

GROMACS provides a tool called ‘g_msd’ to measure diffusion coefficients from the mean square displacement (MSD) of atoms from their initial position ($D = \lim t\to 0 < (x-x_0)^2>/6t$). The 'g_msd' program from GROMACS is used to calculate the mean square displacement (MSD) of buckminsterfullerene atoms from their initial position. This calculation makes it possible to calculate the diffusion coefficient along a simulation. Figure 8 shows the MSD at all simulation time scales for k=1. These figures are in accordance with the results of GROMACS at low times. At short time scales which the inertia dominates the motion and the effect of viscous diffusion can be neglected, the ballistic motion is determined for 0<t<20 ps. The result of the Figure 8 in this domain is comparable with the study of similar simulations for single particle trap in [42].

The diffusion constant for a pure diffusion problem is obtained by fitting a straight line to the rms displacement. As that program uses all starting times, so the number of starting points decays linearly with time. However, the actual sampling decays even more, since for long times, all intervals for different t_0 will partially overlap, while intervals shorter than t_0, are (more) independent.

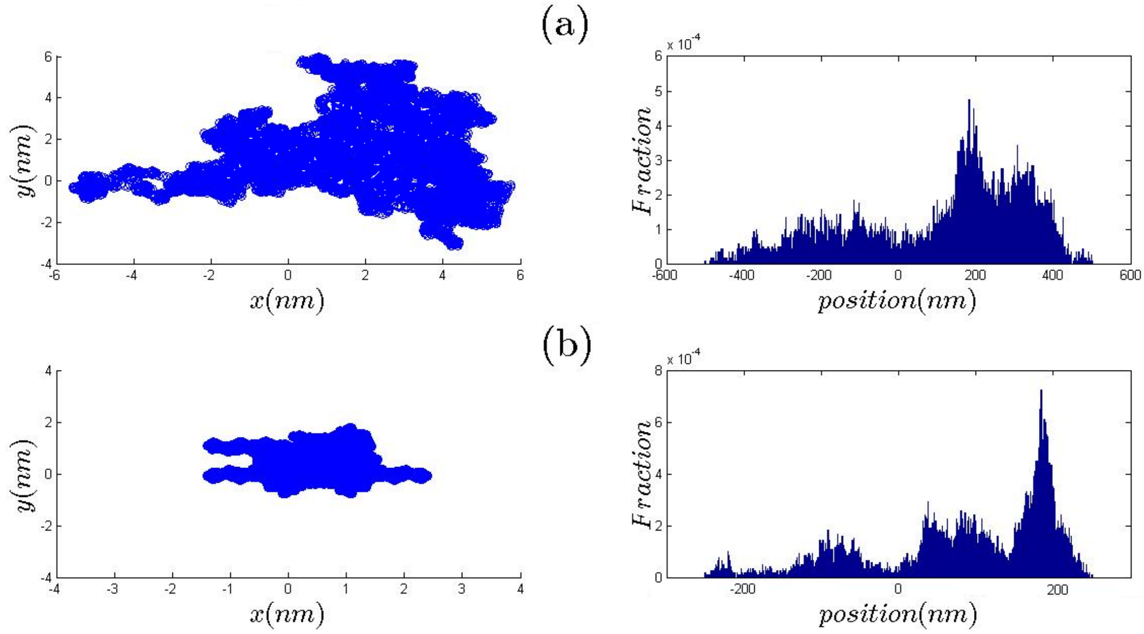

Figure 7. Fraction of buckminsterfullerene position over the time for high and low trap stiffness a) k=0.001 b) k=1

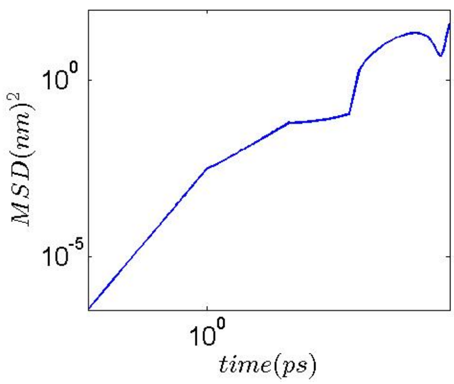

Figure 8. MSD versus time

Table 1. Diffusion coefficient as a function of trap stiffness

case	Appearance (in Time New Roman or Times)	
	k (kJ/mol nm^2)	D (nm^2/ps)
1	10^{-2}	2×10^{-5}
2	2×10^{-2}	2.1×10^{-5}
3	5×10^{-2}	2.3×10^{-5}
4	10^{-1}	8.1×10^{-6}
5	2×10^{-1}	4.1×10^{-6}
6	5×10^{-1}	3.1×10^{-6}
7	1	2×10^{-6}

To obtain the position calibration, the MSD was fitted in the intermediate regime (the regime not yet affected by the trapping potential) with the Hinch [43] theory for a free Brownian particle with the particle radius and a multiplication factor taken as fitting parameters. Table 1 shows the diffusion coefficient as a function of trap stiffness. This table is calculated from the velocity autocorrelation functions. As shown by increase of the trap stiffness the diffusion coefficient decreased. As stated before at fast timescales, the self-similarity of random Brownian motion is expected to break down and be replaced by ballistic motion. So far, an experimental verification of this prediction has been out of reach due to an expense of instrumentation fast and precise enough to capture this motion. At low trap stiffness by MD simulation, here the independence of the diffusion coefficient from trap stiffness is shown in Table 1. So at values less than 50 J/mol/nm^2 for buckminsterfullerene in water, the ballistic motion is observed.

That Table also insists on the fact that the temperature of the buckminsterfullerene is 300 K through the simulation and is independent of the trap stiffness. From the equipartition method, which uses the thermal fluctuation of the particle, for a particle fluctuating in a harmonic potential of the trap and the temperature, the velocity of the particle can obtained. The equation is

$$k_B T = \frac{1}{2} k \bar{x}^2 = \frac{1}{2} m \bar{v}^2 \tag{8}$$

From this fundamental studies on Brownian motion at short time scales of a single Brownian particle, the Maxwell velocity distribution for a nano size particle in a heat bath with constant temperature is verified which confirming the equipartition theorem for a Brownian particle in isotropic Brownian motion in equilibrium systems that has been assumed in theoretical derivations.

4. Conclusions

The simulation and comparing it to the experimental data reveals the basic characteristics of the optical tweezers. The most important results are:

- Angular stiffness of buckminsterfullerene in nano-Optical tweezers can be ignored for practical estimations.
- The Ideal position spectrum of a bead in an optical trap can be used to determine the stiffness of the trap.
- By increase of the trap stiffness, the MSD decreased.
- By increase of the trap stiffness, the maximum distance from the position decreased and the buckminsterfullerene is more confined to the trap center and the trap performance increased.
- Except the beginning of the motion, there is not a significant change in the angular positions of our trapped buckminsterfullerene.
- Ideal position spectrum of a bead in an optical trap can be used to determine the stiffness of the trap.
- The normal distribution of the velocity magnitude around the mean values of it demonstrates the stochastic characteristic of the motion.
- From The equipartition method which uses the thermal fluctuation of the particle, for a particle fluctuating in a harmonic potential of the trap and the temperature, the velocity of the particle can obtained.

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