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Drug Delivery System Model using Optical Tweezer Spin Control

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Abstract

A new concept of molecular motor using optical tweezers within a modified optical add–drop filter known as PANDA ring resonator is proposed. In simulation, dark and bright solitons are input into the system. The orthogonal tweezers can be formed within the system and detected simultaneously at the output ports. Under the resonant condition, the optical tweezers generated by dark and bright soliton pair corresponding to the left-hand and right-hand rotating solitons (tweezers) can be generated. In application, the trapped molecules can be moved and rotated to the required destinations, which can be useful for healthcare applications, especially, in drug delivery, medical diagnosis and therapy.

Keywords: Drug delivery; Molecular motor; Molecular electronics; Optical tweezer; Optical trapping; Optical spin

Introduction

Molecular motor is recognized as an essential agent of living organ movement; especially, for cell communication and signaling. Commonly, cell structure called "cytoskeleton" has a function to serve the track of network in intracellular transport processes and plays a crucial role in a motility of the cell that works as a machine [1,2]. The cytoskeleton within the axon and dendrite cooperating a motor protein can move along the substrate including the actin filament (7 to 9 nm in diameter), microtubule (25 nm in diameter), and intermediate filament (10 nm in diameter) [3]. There are three significant super families of cytoskeleton molecular motor protein, which they are myosin, kinesin, and dynein [4]. The molecular motor manipulation has been extensive investigated by many research techniques, which contributed many advances in studying bio-physical properties of molecular motors [5-7]. In general, the manipulation of molecular motors can be characterized by 5 elements. Firstly, the energy input type supplied to work [8]. Secondly, the type of motion performed by the used components [9]. Thirdly, the monitoring methods used for the operation [10].

Then, it is the possibility of the repeated operation in cycles [11]. Lastly, the average desired time scale to complete a cycle [12]. Furthermore, there are several interesting researches shown that the motor movement direction [13,14] can be controlled, which has been quantitatively analyzed by recording the relative length changes of DNA using laser tweezers or magnetic devices, which allows the individual consecutive chemical and mechanical steps of the motor enzymes to be dissected.

The microscopic manipulation concept was firstly proposed by Ashkin in 1987, which presented the optical trap that became the "optical tweezers" for manipulating biological objects [15], which was shown that bacteria and viruses were trapped using an argon laser at a wavelength of 514 nm. However, the visible laser caused substantial damage to the biological objects even at very low powers. After that, the new era of molecular motor control by light was established, where several studies of different dynamics and bio-molecular processes, ranging from how individual macromolecules such as proteins, DNA, and RNA unfold under force [11,16] was realized, which was shown that how molecular motors translocate and exert forces [17]. The particular interest was that the single-molecule optical trap experiment provided the novel insights into the mechanism of nucleic acid translocate and related researches for trapping nanoparticles [18]. Magnetic tweezers are the interesting techniques to implement for reducing the optical damage induced by in trapped particle [19]. The magnetic tweezers consist of a pair of permanent magnet placing above the sample holder which inverted the microscope outfitted with a charge-coupled device. Magnetic tweezers are capable to form the applied forces of 1 nN, which can be used to manipulate and rotate a magnetic particles ranging from 0.5 to 5 nm. In addition, the tweezer technique can be used *in vivo* of a living organ and fabricated in a nanoscale regime. The technique of Laguerre–Gaussian beam [20] is also available, where all photons have the intrinsic angular momentum called "spin", so a circularly polarized laser beam can also have spin angular momentum. On the other hand, the laser beam with orbital angular momentum can be possibly formed, where the involved torque is strong enough to make the microscopic particle rotation.

In this article, The modified add-drop optical filter known as a PANDA ring resonator has been proposed by Jalil et al. [21] which is capable to generated dynamic optical tweezers (potential wells) in order to trap the nanoparticles. Afterward, a new optical trapping design to transport gold nanoparticles using a PANDA ring resonator system has been reported by Aziz et al. [22], where the intense optical fields in the form of dark solitons can be controlled by Gaussian pulses are used to trap and transport nanoscopic volumes of matter to the desired destination via an optical waveguide. Although, there are many literatures about molecular motor manipulations, but there are rarely researches investigated about molecular motor controlled by light. In this paper, we have demonstrated that the dynamic behavior of the tweezers can be rotated in the same ways as the photonic (optical) spin [23], which can be available for long distance molecule trapping

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and transportation along the optical waveguide, especially, for drug delivery, diagnosis and therapeutic applications [24-26]. Finally, a new concept of molecular motor control using dynamic optical tweezers within a modified optical add–drop filter called PANDA ring resonator is established, the optical tweezers are generated by dark and bright soliton pair corresponding to the left-hand and right-hand rotating solitons. The carrier signals in the form of optical vortices or potential wells can be used to trap and rotate molecules by the plasmonic surfaces and transport along the optical waveguide. The merit of such system is highly stable signal with no fluctuation over a certain period of time, where the trapped atom or molecule is confined during the delivery process. More recently, the interesting works are given in details in the conclusion section, where in application the trapped molecules can moved and rotate to the required destinations, which can be useful for many applications, especially, for drug delivery, medical diagnosis and therapy.

Molecular Motor Mechanism

Generally, myosin moves on the actin filaments, while both kinesin and dynein move on the microtubules. Most of these molecular motors are dimers with two 'heads' connected together at a 'stalk' region and a 'tail' domain opposite the heads. The head of the molecular motor contains the motor domain that provides the motion along the filaments whereas the tail of the molecular motor contains the subunits responsible for cargo binding and regulation. Molecular motor can take hundreds of steps along the respective filament in long-distance cellular cargo transport before detaching. Some cargos such as vesicles, mitochondria, mRNA, virus particles, and endosomes [27] are moved by such motors. The movement of kinesins is in a hand-over-hand mechanism, which is interesting to be more understood [12]. Dynein molecular motors are divided into two groups: (i) cytoplasmic dyneins which achieve various intracellular cargo transport functions; and (ii) axonemal dyneins which powers the motion of cilia and flagella in some eukaryotic cells and are attached in large linear arrays along the microtubule inside the cilia and flagella. All dyneins walk toward the minus-end of microtubule. By using an electron microscopy, it utilizes the reconstructions of cytoplasmic dynein demonstrate a structure similar to axonemal dynein. Hence, the inducement of mechanical torque of their functions occurs in a similar way [28]. The myosin molecular motors function in a variety of cellular tasks, from cellular transport to muscle contraction. Consequently, the myosins are divided into two groups: (i) non-muscle myosins which are involved in organelle transport along actin filaments very similar to the mechanism of kinesins; and (ii) muscle type myosins that drive muscle contractions and is an important component of the muscle. These cellular movements, cellular transport and muscle contraction, depend on the interactions between actin filaments and myosin [29]. The transportation process is vital for cell because it confines selected organelles with appropriate spatial-temporal coordinates. Currently, variety of research on motor performance focuses on mechanochemical cycle to perform mechanical movements under control of appropriate energy inputs [30] and duration of the motor protein along the substrate in the average forward moving [31].

Figure 1 shows the axonal transports of membranous in vivo, where the cross bridge structures between microtubules and membranous organdies have identified by the electron microscopic technique which candidates for membranous organelle translocations. At present, kinesin and dynein have been well-known in neurons as microtubule motors that produce the force necessary for the fast axonal transport of membranous organelles. Dyneins can move toward the minus end of the microtubule, where they transport cargo from the cell margin toward the centre from the neuronal axon terminal to the cell body (soma), which is known as retrograde transport. A different type of motor protein known as kinesin moves to the plus end of microtubules, which is associated with the anterogradely moving membranous organelles in the axon, so it is considered to be an anterograde translocation. The microtubule structure is seen in the polar form and the head only connected to the microtubule in one orientation, while the ATP binding gives each step of its direction through a process called neck linker zippering as shown in Figure 2.

The conventional kinesin and other members of the kinesin family bind ATP and microtubules at specific site in their conserved motor domain, and use the energy from ATP hydrolysis to produce force and move along the microtubules. There are 45 different kinesin species in humans, where they can be distributed in all eukaryotic cells by linear motors, which are involved in many functions of biological systems, including cargo transport, microtubule dynamics control, mitosis and they play a crucial role in signal communication ways. Kinesins have a wide variety of structures, and they function as monomers, dimers, or tetramers in cells, which are classified into three categories: N-terminal kinesins, C-terminal kinesins, and M-kinesins. N-terminal kinesins move to the plus end of the microtubule, and C-terminal kinesins move toward the minus end of the microtubule [12]. When the kinesin motor and microtubule track interacted, the bead is pulled along by the kinesin and the nanometer scale displacements, in which the volume with variety of vesicle pore size is within the range of 10-400 nm.

Molecular Motor Control

Light carrier known as an optical tweezer can be utilized to the exert force on a microscopic object, where a restoring force proportional to the displacement of the microsphere is introduced. An optical trap or "tweezer" is an all-optical non-contact tool, which is grounded on a strongly focused laser beam to trap a dielectric object near the focal point [32]. In principle, the momentum transfer is associated with bending light as the quanta of light energy proportional to its momentum and in the direction of propagation. The momentum of the light refracts and changes direction when light passes through an object [33]. To conserve the total momentum, an object acquires momentum equal to that lost by the photons, in which the sum of forces can be separated into two components, the scattering force, in the direction of incident light and the gradient force arises from the intensity gradient pointing toward the center of the beam [34,35]. In this work, a static

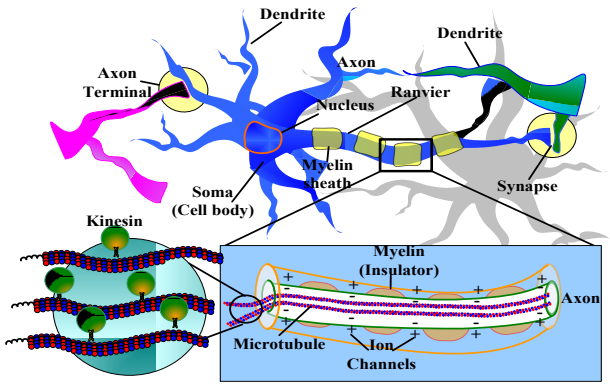

Figure 1: Axonal transport model of membranous organelle for cell communications

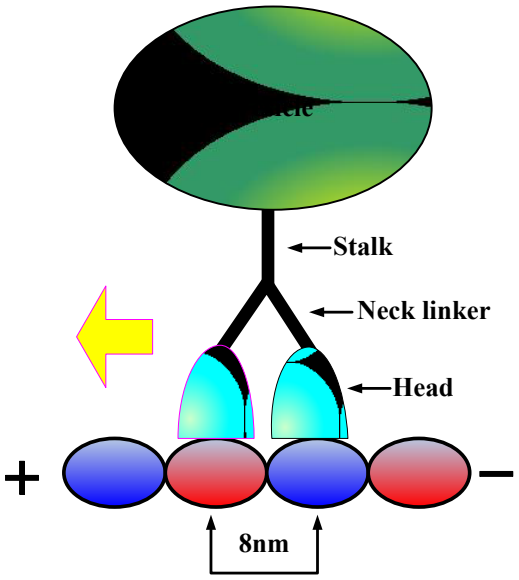

Figure 2: Schematic of gross anatomy of a kinesin motor protein

optical tweezer act on the object is demonstrated as illustrated in Figure 3, which is used to move kinesin motor along microtubule filament. More details of potential wells or dynamic tweezers are found in [36]. The trapping phenomenon is categorized into two types as Rayleigh trapping and Mie trapping, which can be used to hold and move microscopic dielectric objects physically with following details. If the size (d) of the trapped particle is much smaller than the wavelength of the trapping beam (d<<λ), such trapping is known as trapping in the Rayleigh regime. The force performing on the particles can be considered as a miniscule dipole immersed in the optical trapping field oscillating at frequency ν. The two forces acting on the particles are known as dipole scattering and Lorentz force (gradient force). In Mie trapping, the size of the trapped particle is larger than the wavelength (d>>λ). In this paper, the Rayleigh trapping is described in detail because the molecular motor diameters are much smaller than the carrier signal wavelength. The optical force on the trapped particle can be defined and found in [37].

$$F = \frac{Qn_m P}{c} \tag{1}$$

Q represents the fraction of power utilized to exert force, which is equal to 1, known as dimensionless efficiency, n_m is the refractive index of the suspending medium, P is the incident laser power, measured at the tested sample or volume and c is the light speed. For plane wave incident on a perfectly absorbing particle to achieve stable trapping, the radiation pressure must create a stable and three-dimensional equilibrium. As biological specimens are usually immersed in an aqueous medium, the dependence of force F on n_m can be used to achieve higher trapping forces. Q is therefore the main determinant of trapping force and depends upon the numerical aperture (NA), laser wavelength, laser mode structure, relative index of refraction, light polarization state, and particle geometry. The scattering force is given by [37]

$$F_{scatt} = n_m \frac{P\langle S\rangle \sigma}{c} \tag{2}$$

where

$$\sigma = \frac{8\pi r^2 (kr)^4}{3}\left(\frac{m^2-1}{m^2+2}\right)^2, \tag{3}$$

Here P is the incident laser power intensity by optical spin, σ is the scattering cross section of a Rayleigh sphere with radius r. $\langle S\rangle$ is the time averaged Poynting vector, n is the index of refraction of the particle, $m=n/n_m$ is the relative index, and $k=2\pi n_m/\lambda$ is the wave number of the light. The scattering force is proportional to the energy flux and points along the direction of propagation of the incident light. The scattering force is proportional to the energy flux and points along the incident light propagation direction.

The time averaged gradient field is the Lorentz force performing on the dipole induced by the light field given by [37].

$$F_{grad} = \frac{2\pi\alpha}{cn_m^2}\nabla\langle P\rangle \tag{4}$$

where

$$\alpha = n_m^2 r^3\left(\frac{m^2-1}{m^2+2}\right) \tag{5}$$

The gradient force is proportional to the intensity gradient and points up the gradient when m>1. From equations (4) and (5), the large gradient force can be obtained by the large depth of the laser beam, in which the stable trapping force requires the gradient force in the $-\hat{z}$ direction against the direction of incident light (dark soliton valley) as shown in Figures 5 and 6. The gradient field strength can be increased by increasing in the laser beam Numerical Aperture (NA) and decreasing in focal spot size. In principle, the potential well is produced among the gaps by two forces to confine the trapped volumes.

Simulation Results

The optical manipulations in many substances are based on optical dipole interaction model, where photon from source can result in serious effect when light is interacting in nanoscale structure. Optical dipole is formed by spin manipulation, where the dark-bright soliton conversion behaviors can be controlled by using a ring resonator [24]. The PANDA ring resonator is used to form the orthogonal set of dark-bright soliton pair, which can be decomposed into left and right circularly polarized wave [24]. The two output light signals relative in phase after coupling into the optical coupler is π/2. So, the signals coupled into the Drop Port (Dr) and Through Port (Th) has a phase difference of π with respect to the Input Port (In) signal. The output powers at the drop and through ports are given by [24].

$$\left|E_d\right|^2 = \left|\frac{-k_1 k_2 A_{1/2}\Phi_{1/2}}{1-\tau_1\tau_2 A\Phi}E_i + \frac{\tau_1\tau_2 A\Phi}{1-\tau_1\tau_2 A\Phi}E_a\right|^2 \tag{6}$$

$$\left|E_t\right|^2 = \left|\frac{\tau_2-\tau_1 A\Phi}{1-\tau_1\tau_2 A\Phi}E_i + \frac{-k_1 k_2 A_{1/2}\Phi_{1/2}}{1-\tau_1\tau_2 A\Phi}E_a\right|^2 \tag{7}$$

Here $A_{1/2}=\exp(-\alpha L/4)$ (the half-round-trip amplitude), $A=A_{1/2}^2$, $\varphi_{1/2}=\exp(j\omega T/2)$ (the half-round-trip phase contribution), and $\varphi=\varphi_{1/2}^2$

In simulation, the orthogonal soliton sets can be generated by using the system as shown in Figure 4. The optical field is fed into the ring resonator system, where $R_1=R_2=2.5$ μm, $R_{ad}=30$ μm by using a microring, $R_c=20$ μm. To form the initial spin states, the magnetic field is induced by an aluminum plate coupled on ***AlGaAs***

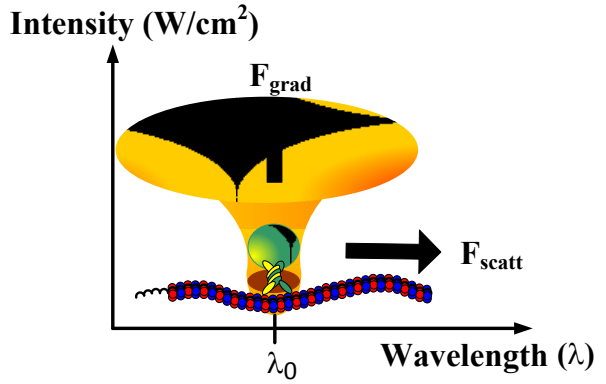

Figure 3: The optical forces is formed by a potential well, which is generated by a dark soliton.

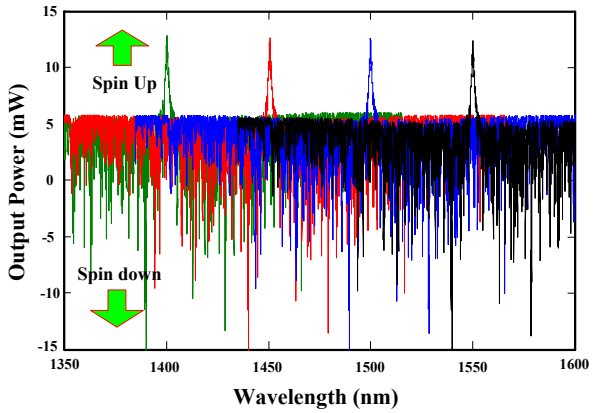

Figure 4: Photonic spins are generated and confirmed by using a PANDA ring [24].

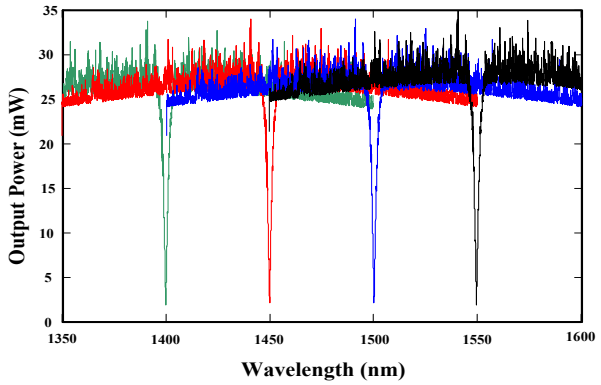

Figure 5: Optical tweezers with different wavelengths generated by dark-bright soliton pair [24]

waveguides for optoelectronic spin-up and spin-down states. The coupling coefficient ratios κ_1:κ_2 are 50:50, 90:10, 10:90 and κ_c are 50:50. The system parameters are the ring radii R_{ad}=300 nm, A_{eff}=0.25 μm², n_{eff}=3.14 (for InGaAsP/InP) [24], α=0.1 dB/mm, γ=0.01, λ_0=1.45 μm. The output intensities of spin-injected for Transverse Electric (TE) and Transverse Magnetic (TM) fields are generated by using a PANDA ring resonator. The optoelectronic fields are generated by a dark-soliton pump based-on through port and drop port microring resonator at center wavelength 1.45 μm. The random Transverse Electric (TE) and transverse magnetic(TM) fields of the solitons corresponding to the left-hand and right hand photons can be generated and simulated by using the Optiwave and MATLAB programs [24]. The angular momentum of either + ħ or –ħ is imparted to the object when a photon is absorbed by an object, where two possible spin states known as optoelectronic spins are exhibited. Many soliton spins can also be generated and detected at through (spin up) and drop (spin down) ports of a PANDA ring resonator in Figure 4. The optoelectronic spin manipulation generated within a PANDA ring resonator as shown the dipole pair with wavelength was varied. Therefore, the output signals of spin optical tweezers by four wavelengths were produced in PANDA ring resonator is obtained at the Th and Dr ports as illustrated in Figure 5.

The important aspect of this simulation is that the required dynamic behavior of the tweezers can be obtained by tuning some parameters of the system including add port input signal, coupling coefficient, and ring radius. In this study, it is adapted by using a microtubule inserting into an *InGaAsP/InP* waveguide of microtubule filament as shown in Figure 6, which consists of two states. Firstly, a device called a "PANDA ring resonator" is used to generate the spin potential well for molecule trapping. Secondly, the trapped molecules can be moved and rotated to the required destination by the generated potential wells.

The kinesin and molecule transportation manipulations are as shown in Figure 6, where the waveguide is connected to the microtubule of neuronal cells, in which the microgel/nanogel is used to connect the waveguide all the way through the neuronal cells. In addition, an array of molecules can be used to trap and rotate many molecules, which can be used to form large scale molecular spins (molecular motors), in which the different sizes of trapping forces are generated, which is allowed to form the different molecular motor sizes, which can be useful for many applications, especially, in drug delivery, medical diagnosis and therapy.

Conclusion

We have demonstrated that the molecular motors using optical tweezers within a modified optical add–drop filter known as PANDA ring resonator can be generated and performed. In simulation, the orthogonal tweezers can be formed within the system in the same way as photonic spins, in which the rotated tweezers can be generated and controlled. Simulation results have shown that the spin tweezers with the trapped molecules can be rotated (molecular motors), controlled and moved along the specific waveguide by the plasmonic surfaces,

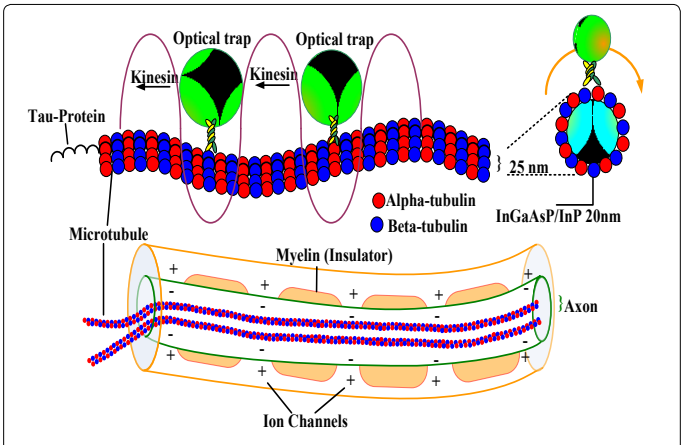

Figure 6: Molecule movement by molecular motor to the required destinations

as shown in Figure 6 to the required destinations, which is allowed to reach the required drug targeting or therapeutic access points. Furthermore, the molecular motor array, i.e. many trapped molecules can be generated and moved by using the proposed system, which can be used to form large scale molecular motors use, which is useful for healthcare technologies, especially, drug delivery, medical diagnosis and therapy, in which the required therapeutic targets or accessed points can be controlled realized. The promising applications of drug delivery using the rotation concept are also found in the recent published works [38,39].

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