FDTD simulation of trapping nanowires with linearly polarized and radially polarized optical tweezers

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Abstract: In this paper a model of the trapping force on nanowires is built by three dimensional finite-difference time-domain (FDTD) and Maxwell stress tensor methods, and the tightly focused laser beam is expressed by spherical vector wave functions (VSWFs). The trapping capacities on nanoscale-diameter nanowires are discussed in terms of a strongly focused linearly polarized beam and radially polarized beam. Simulation results demonstrate that the radially polarized beam has higher trapping efficiency on nanowires with higher refractive indices than linearly polarized beam.

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OCIS codes: (140.7010) Laser trapping; (350.4855) Optical tweezers or optical manipulation.

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1. Introduction

Optical tweezers have become important and commonly used tools in the field of physics and life science for trapping and moving objects ranging in size from tens of nanometres to tens of micrometres [1,2] since their introduction in 1986 [3]. Recently, Optical tweezers have been used to trap and process nanowires and other nanomaterials to build new types of micro-nano

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devices [4–6]. However, most materials used for nanowires have high refractive indices, which cause difficulty in trapping by optical tweezers.

The radially polarized beam is a kind of center hollow beam, and the energy of the beam is distributed at the fringe of the beam, which is an advantage for the reduction of scattering force on the nanowire and the improvement of gradient force. In addition, the radial polarization also contributes to the improvement of gradient force. Here the trapping capacity on nanowires with the radially polarized beam is simulated and compared with that of conventionally linearly polarized beam.

For the diameter and length of nanowires in the simulation model both are between 0.1λ~10λ (λ is beam wavelength). Direct solutions of Maxwell's equations are suitable to get the electromagnetic field, and then the force on a nanowire can be calculated from the Maxwell stress tensor or Poynting's vector method. In this regard the T-matrix method has been used to simulate laser trapping of nanorods with a circularly polarized beam [7] and linear nanostructures composed of identical nano-spheres with a linearly polarized beam [8]. The three dimensional finite-difference time-domain (FDTD) method is also a robust approach to solve Maxwell's equations. Although this method is time-consuming, it is very powerful with the potential to model arbitrary shaped objects and different traps. Therefore, in our work a three dimensional FDTD is used to setup a numerical simulation model.

2. Calculation

2.1 Setting of beam

The vector spherical wave functions (VSWFs) are a complete and orthogonal set of solutions to the vector Helmholtz equation [7,9]. For tightly focused beams, the fifth-order Gaussian beam description provides a significantly improved solution to Maxwell's equations in comparison with commonly used paraxial Gaussian beam descriptions [10]. In order to accurately simulate the transmission form of electromagnetic field, the VSWFs are adopted to express fifth order Gaussian beams as incident light [9–13].

$$\mathbf{E}_{inc} = \sum_{n=1}^{\infty} \sum_{m=-n}^{n} [\mathrm{a_{mn}} \mathrm{Rg}\mathbf{M}_{mn}(\mathrm{k}\mathbf{r}, \theta, \varphi) + \mathrm{b_{mn}} \mathrm{Rg}\mathbf{N}_{mn}(\mathrm{k}\mathbf{r}, \theta, \varphi)] \tag{1}$$

$$\mathbf{H}_{inc} = -\mathrm{j}\sqrt{\frac{\varepsilon}{\mu}} \sum_{n=1}^{\infty} \sum_{m=-n}^{n} [\mathrm{b_{mn}} \mathrm{Rg}\mathbf{M}_{mn}(\mathrm{k}r, \theta, \varphi) + \mathrm{a_{mn}} \mathrm{Rg}\mathbf{N}_{mn}(\mathrm{k}\mathbf{r}, \theta, \varphi)] \tag{2}$$

In the above formulae k is wave number, a_{mn} and b_{mn} are shape coefficients, $Rg\mathbf{M}_{mn}$ and $Rg\mathbf{N}_{mn}$ are vector wave functions based on spherical coordinates. In the case of x linearly polarized beam, m = 1 and −1,

$$a_{1n} = a_{-1n} = -b_{1n} = b_{-1n} = -(-i)^{n+1}[4\pi(2n+1)]^{1/2} g_{5,n} \tag{3}$$

$$\begin{aligned} g_{5,n} = \exp[-s^2(n-1)(n+2)\{1+(n-1)(n+2)s^4[3-(n-1)(n+2)s^2]+ \\ (\mathrm{n}-1)^2(\mathrm{n}+2)^2 s^8[10-5(\mathrm{n}-1)(\mathrm{n}+2)s^2+0.5(\mathrm{n}-1)^2(\mathrm{n}+2)^2 s^4]\}, \end{aligned} \tag{4}$$

$$\mathrm{s} = 1/\mathrm{k}\omega_0 \tag{5}$$

Here $g_{5,n}$ are coefficients for fifth order Davis beam [9], s is the dimensionless beam shape parameter, ω_0 is the beam waist radius, n is the number of spherical wave. As $n \geq 30$, the numerical error is negligible [12], so $n = 30$.

In the case of radially polarized beam,

$$\mathbf{E}_{\mathrm{inc}}^{\mathrm{r}} = \mathbf{E}_{inc} \cdot r_{\mathrm{inc}} \tag{6}$$

$$\mathrm{H}_{inc}^{r} = \mathrm{H}_{\mathbf{inc}} \cdot \mathbf{r}_{inc} \tag{7}$$

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Here rinc is radial position vector matrix in the incident plane of the beam. The TM components of formulas (6) and (7) represent a radially polarized beam [14,15]. Figure 1 shows the normalized intensity distribution in the focal plane of linearly polarized beam and radially polarized beam respectively.

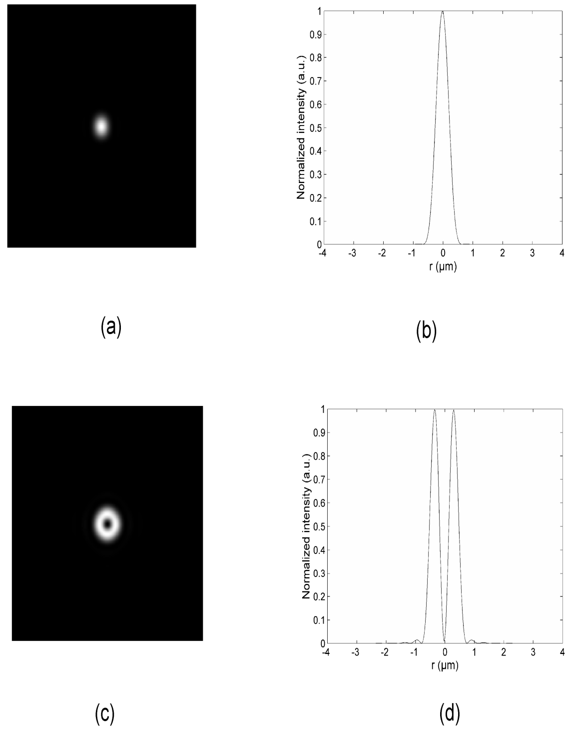

Fig. 1. The normalized intensity distribution in the focal plane. (a)linearly polarized beam; (b)the radial cross section of linearly polarized beam; (c)radially polarized beam; (d)the radial cross section of radially polarized beam.

2.2. Calculation of optical trapping force

The electromagnetic force on a nanowire in a medium can be obtained by the Maxwell stress tensor.

$$\mathbf{F} = \int_S < \mathbf{T} > \cdot \mathrm{d}\mathbf{S} \tag{8}$$

T is Maxwell stress tensor,

$$\langle T \rangle = \frac{1}{2} \mathrm{Re} \left[\varepsilon E E^* + \mu H H^* - \frac{1}{2} (\varepsilon E^2 + \mu H^2) n \right]. \tag{9}$$

The bracket < > denotes time averaged value, $d\mathbf{S}$ is the unit normal to the nanowire's surface, ε is the permittivity of the background medium, μ is the permeability of the background medium, **n** is the normal vector of the nanowire's outer surface, **E*** and **H*** represent the complex conjugates of the electric and magnetic field.

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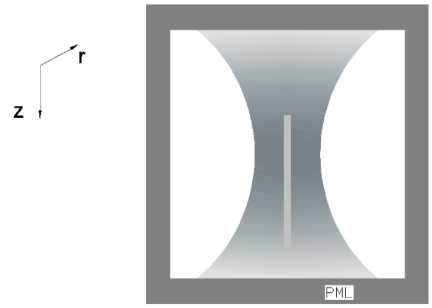

Fig. 2. Computational domain.

3. Results

Simulations were performed on the computer with dual-core CPU E5200 and 4.0G Memory. Matlab language is used for programming. In the model the size of the lattice can be 250 × 250 × 220, the cell size is not greater than λ/20, PML (Perfectly Matched Layer) absorbing boundary is adopted. Figure 2 demonstrates a calculation region for single optical tweezers to trap a nanowire in water with the beam propagating along the z axis, in the z direction. The radial direction r is perpendicular to the z axis. The nanowire has a cylindrical shape with a radius of 60nm and a height of 2100nm, its refractive index is 1.6. The trapping beam with a wavelength of 600nm, a waist radius of 300nm and a power of 10mW is linearly polarized and radially polarized respectively.

As single optical tweezers trap a nanowire, the nanowire orients itself to the optical axis of the beam (Fig. 2). The axial force efficiency Q_z ($Q = Fc/(np)$, c is the speed of light, F is the trapping force, n is the refractive index of the background medium, p is the beam power.) and radial force efficiency Q_r are shown in Fig. 3. In the following figures the abscissa denotes the displacement of the geometrical center of nanowire from the focus and the ordinate represents force efficiency. Figure 3(a) shows that there is little difference between the maximal axial forces of the linearly polarized beam and these of the radially polarized beam, the axial trapping positions in both beams are located behind the focus. The maximal radial forces of the radially polarized beam are obviously greater than those of the linearly polarized beam (Fig. 3(b)), the radial forces of the radially polarized beam near the focus appear to fluctuate and there is more than one radial equilibrium position existing.

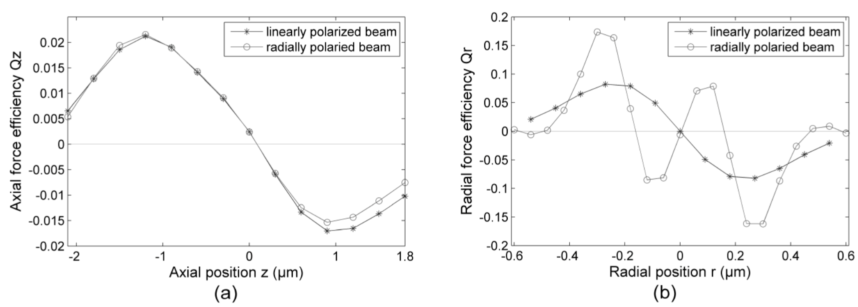

Fig. 3. Axial (a) and radial (b) forces on nanowire with refractive index of 1.6 as a function of nanowire's displacement from the focus. The asterisk represents linearly polarized beam, the circle denotes radially polarized beam.

As the nanowire's refractive index is 2.5, the obtained forces are shown in Fig. 4. It can be seen that the axial forces and radial forces of radially polarized beams increase greatly compared with those of linearly polarized beams. It is due to the hollow beam and

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polarization singularity of radially polarized beams, which decrease radiation pressure forces on nanowire and improve gradient forces.

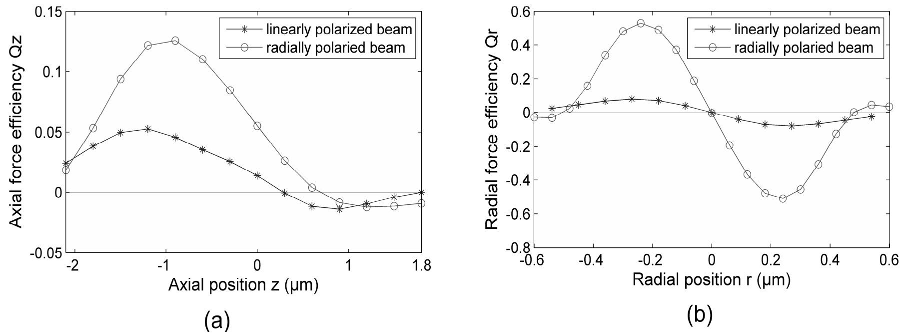

Fig. 4. Forces on nanowire with refractive index of 2.5.

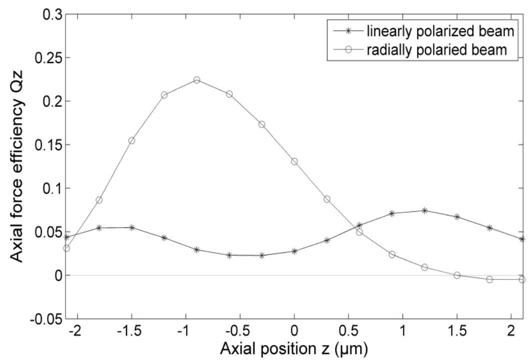

Fig. 5. Axial forces on nanowire with refractive index of 3.0.

As the nanowire's refractive index is 3.0, it is infeasible for a linearly polarized beam to trap nanowires along axial direction in the vicinity of the focus (shown in Fig. 5). However, trapping is achievable for radially polarized beams and the axial trapping position is located 1.5μm behind the focus. The axial trapping potential corresponding to the area under the curve $Q_z\ (z)$ is defined as $U(z) = -\int F_z dz = -(np/c)\int Q_z dz$ [7], which represents the energy required for nanowires to escape from the trap. Although the axial trapping potential of radially polarized beam in Fig. 5 is of pronounced asymmetry with respect to the equilibrium position $Q_z = 0$, the energy barrier in the beam propagating direction is significantly larger than the thermal energy $k_B T$ (k_B is the Boltzmann constant, T is the temperature of the background medium, $T = 300K$).Therefore, it is difficult for nanowires to escape from the trap by the Brownian motion.

4. Conclusions

The three dimensional FDTD method and Maxwell stress tensor are used to setup simulation model and calculate the trapping force. By using VSWFs the transmission fields are obtained with linearly polarized and radially polarized beams in the vicinity of focus point. The trapping capacities on nanoscale-diameter nanowires based on both linearly polarized beam and radially polarized beam are simulated and compared with each other. When radially polarized beam is adopted for lower refractive index nanowire, the multiple trapping equilibrium positions beyond the focal plane exist. With the increase of the refractive indices of nanowires, the axial and radial forces of the radially polarized beam both increase greatly. The radially polarized beam, compared with the linearly polarized beam, demonstrates higher

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trapping efficiency on the higher refractive index nanowire. It is shown that the radially polarized beam is suitable for trapping those higher refractive index nanowires.

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