Validity of cylindrical approximation for spherical birefringent microparticles in rotational optical tweezers

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Abstract
Rotational manipulation of microscopic birefringent particles has conventionally been done by manoeuvring the polarization of the trapping light in optical tweezers. The torque on the particle is a sum of contributions from the linear polarization and the circular polarization, while assuming that the difference in optical path lengths between the extraordinary and the ordinary components of polarization depends upon the wavelength of light, the thickness of the particle and the birefringence. Generally, the thickness of spherical microparticles is assumed to be the diameter which renders the particle appear cylindrical. We find that for a range of particles from the Rayleigh regime to the early Mie regime, the approximation holds good.

1. Introduction
Rotational micromanipulation holds tremendous importance addressing some of the motional degrees of freedom of a rigid body. People have used many tools to rotate particles in the mesoscopic domain, namely optical tweezers [1, 2], magnetic tweezers [3], rotation of micropipettes [4], optically induced forces [5], lever action rotation [6], active motion of particles [7] and so on. Among these, the rotation induced by the optical tweezers preferentially relies on use of birefringent probes which can then be addressed by polarized light [1, 2, 8–10].

The polarization of light interacts with the two different refractive indices offered by the particle in two directions to generate a torque depending upon the difference in optical path lengths. A typical particle which has been assumed to be spherical for the purposes of Stokes drag [1, 2, 8, 11] would then need to be assumed as cylindrical so as to assume uniformity over the entire cross-section. Thus, a spherical particle then requires to be assumed cylindrical. It is this assumption that we investigate in this manuscript.

The problem of calculating the scattered light from a spherical birefringent microsphere is complicated due to the lack of a birefringent theory for Mie scattering. These have sometimes been modelled as a large sphere with an enclosed spherical void which is eccentrically displaced [12]. But these do not capture all the features of the light scattered from the particle. We consider a birefringent particle as belonging to a certain shape with a void filled with a different material but ellipsoidal in shape to generate birefringence. This kind of a model has successfully generated the four lobe backscatter pattern under crossed polarizers [13]. We consider the torques generated on such particles with a cylindrical outer shape compared to that for a spherical outer shape and ascertain the ratio of the effective diameters that appear in the effective path lengths. and relate with the assumed birefringence due to ellipsoidal void. We find that the cylindrical approximation is good for spherical particles in the Rayleigh regime and the early Mie regime with some changes for higher particle dimensions.
2. Theory

The torque between the polarized light and the birefringent microparticle can be written as \[ \tau = -\frac{\epsilon}{2\omega} E_0^2 (A - B) \] (1)

\[ A = \sin(kd(n_0 - n_e))\cos(2\phi)\sin(2\theta) \] (2)

\[ B = [1 - \cos(kd(n_0 - n_e))]\sin(2\phi) \] (3)

Here, \( \epsilon \) indicates the permittivity of the material, \( \omega \) the frequency of light, \( k \) the wave vector, \( d \) the diameter of the material and \( (n_0 - n_e) \) the birefringence of the material. The angle \( \phi \) indicates the ellipticity of the light, while the angle \( \theta \) is the angle between the direction of linear component of polarization of light with the director of the birefringent particle. \( E_0 \) is the electric field of the light. Thus, the torque depends upon differential optical path length encountered by the two different polarizations of light as these pass through the material, \( k d (n_0 - n_e) \). This expression was derived for a cylindrical particle. Ever since this phenomenon was observed, people have assumed that the optical thickness of the particle can be approximated to be that of a cylindrical particle irrespective of the shape of the actual particle. Even spherical particles, which have mostly been considered for rotational micromanipulation, have also been assumed to be cylindrical for the purposes of calculating the torque.

In order to perform the simulation, which we perform in the numerical software using the FDTD technique, we assume that the birefringent microparticle is composed of a sphere of some refractive index with an ellipsoidal void filled up a material of a different refractive index \[ \ref{13} \]. This appears to be a good approximation as the liquid crystal directors inside a typical liquid crystalline birefringent microsphere anyway align in ellipsoids such that the effective single ellipsoid placed at the middle of the particle seems to have an equivalent form birefringence corresponding to the entire real particle \[ \ref{15} \]. These particles become birefringent by picking up a bipolar director configuration. We can represent many such ellipsoidal surfaces by one single ellipsoid with a representative refractive index and form birefringence to give an equivalent birefringence. The same logic applies to vaterite particles which have hyperboloid director surfaces defining the birefringence.

The diameter of the sphere and the major axis of the ellipsoid are considered to be same, while we vary the semi-minor axis of the ellipsoid to generate various birefringences. We assume here that the form birefringence of the material depends upon the ratio of the semi-major axis to semi-minor axis while being independent of size \[ \ref{16} \]. We compare this sphere-void system to a cylinder-void system which has both the height and the diameter of the face equal to the diameter of the sphere, shown in figure 1.

We calculate the torque on the microparticle by using the Maxwell Stress Tensor performed in Lumerical on an imaginary box surrounding the particle.

\[ \tau_i = \int_{S_i} \epsilon_{ij} r_j \sigma_{kl} dS_l \] (4)

where, \( \sigma_{ij} \) is the Maxwell Stress Tensor \[ \ref{17} \]. The particles are depicted in figure 1, where, in (A), a cylindrical particle with an ellipsoidal void has been shown which describes a birefringent particle well, while on the (B) is a spherical particle with similar dimensions with just the shape changed. We apply a plane wave with elliptically polarized light to this system and then find the torque out from equation (4). The Maxwell Stress Tensor
computation is independent of the choice of the imaginary surface, which we consider to be cubical to use cartesian coordinates.

Now the potential that the particle sees while trying to rotate is given by the washboard potential [14]. If $\theta$ is held at 45 degrees, when the linear restoring component of the torque is maximum, a typical response given by equation (1) as a function of ellipticity angle $\phi$, is shown in figure 2.

The value of $\phi$ where the torque goes to zero can be found as [18],

$$\phi_{tr} = \frac{\pi - kd(n_e - n_i)}{4} \quad (5)$$

so that the effective diameter $d$ for each shape is given as

$$d = \frac{\pi - 4\phi_{tr}}{k(n_e - n_i)} \quad (6)$$

Thus, assuming that both the types of particles have the same birefringence, coming from the identical ellipsoidal void, giving the same value of $n_e - n_i$, the correction factor for the diameter of the sphere as compared to the thickness of the cylinder can then be written as

$$\frac{d_p}{d_{cy}} = \frac{\pi - 4\phi_{tr}}{\pi - 4\phi_{cy}} \quad (7)$$

3. Simulation

We make a plane wave of controlled ellipticity incident on a particle along the z direction and subsequently compute the electric and magnetic field in the neighborhood. We define a test box of fixed dimension for all particles and compute the torque in accordance with the equation (4) by considering the various components of the electric and magnetic fields on the sides of the test box. The final torque due to each ratio of semiminor to semimajor axis of the ellipsoid constructed inside the sphere of figure 1 for different values of ellipticity of the incident light is recorded. A typical curve for the ratio to be 0.6 has been shown in figure 2. The red curve indicates the sphere while the blue curve indicates the cylinder. The intercepts to the torque value of 0 were then interpolated using local straight line fits and then the ellipticity angle for the vanishing of torque estimated.

Thereafter, we use the equation (7) to find the ratio of the apparent thicknesses for the sphere and the cylinder. The wavelength of the plane wave was assumed to be 1 $\mu$m. The subsequent ratios were then plotted as a function of the size in figure 3.
4. Results and discussions

We find that the ratio of the apparent diameter of the sphere compared to the cylinder remains at 1 irrespective of the size of the particle, particularly in the Rayleigh and early Mie regimes (shown in figure 3), till an outer diameter of 1 μm of the particle. This indicates that assuming a cylindrical shape for a spherical particle does not make much difference to the computed torque.

Since we compute the ellipticity of light for which torque vanishes using this approach, the exact amplitude of the electric field of incident plane wave is immaterial.

In an optical tweezers, a beam of light is focused very tightly to form a spot of high intensity, whereafter the light diverges again. By the principles of Gaussian beam propagation, there is a region of the beam where the light is almost plane parallel, known as the Rayleigh range. It is here that the beam intensity is the maximum and where the particle is trapped. For a typical 1064 nm trapping laser, the Rayleigh range extends over 3 to 4 microns, such that irrespective of the tight focusing, the plane wave is a good approximation for the incident light. An extensive computation can be made using the angular spectrum method \[19, 20\] which does indicate that under standard configurations of optical tweezers, the focal spot has a high radius of curvature, not to mention the polarization also being the same as the input polarization. Imperfections to the polarization only starts to appear away from the focus.

If we assume that the particle is oriented along the x-y plane while the incident plane wave is not emerging from z direction but at some angle from it, the problem can be mapped to the case when the incident plane wave is along z axis while the birefringence axis is tilted from the x-y plane. We have only considered elliptical polarization along the x-y plane and no components along x-z or y-z planes. Thus the out-of-plane polarization in x-z plane is still along the x axis. This generates a restoring torque along the x-z plane to orient the particle along the x-y plane only. Thus, we can safely ignore the other incident angles for torque computation in x-y plane. Thus this case is only practically relevant.

5. Conclusions

We establish that corrections to the apparent diameters for the spherical particles are not required while computing the torque towards optical tweezers. This is relevant for precision calculations of torque for various applications wherever rotational optical tweezers can be used.

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