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Tilt angle dependent three-dimensional-position detection of a trapped cylindrical particle in a focused laser beam

Holger Kress, Ernst H. K. Stelzer, and Alexander Rohrbach
European Molecular Biology Laboratory (EMBL), Meyerhofstrasse 1, Postfach 10.2209, D-69117 Heidelberg, Germany

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We investigated theoretically the applicability of an optically trapped cylindrical particle as a local probe in photonic force microscopy. To do this we calculated the far-field scattering from a subwavelength-sized dielectric cylinder in a highly focused laser field. From this we obtained interferometric three-dimensional-position detection signals and compared these to signals calculated for a spherical particle. We have calculated the accuracy to which the position of an optically trapped cylinder can be determined, as a function of the cylinder’s orientational fluctuations. The position accuracy is better than a few nanometers for tilt angle fluctuations up to several degrees. Our study is relevant for trapping experiments, where the influence of angle fluctuations needs to be estimated. © 2004 American Institute of Physics.

In a photonic force microscope (PFM), an optically trapped particle acts as a probe which, driven by Brownian motion, scans its local environment. The interaction between probe and environment is determined by measuring the probe’s fluctuations. The principle of the PFM is illustrated in Fig. 1: An objective lens (OL) with a high numerical aperture (NA) focuses a laser beam and thereby creates an optical trap for a particle in the focal region. If the probe is spherical (bead), the particle’s three-dimensional (3D) position is measured with nanometer precision using a quadrant photodiode (QPD), which is placed in the back-focal plane (BFP) of the detection lens (DL) or at a conjugate plane. Linear combinations of the four QPD signals yield the two lateral position signals \( S_x \) and \( S_y \), and the axial position signal \( S_z \). These signals are linear functions of the bead’s position in a restricted region. In common optical trapping schemes with dielectric micrometer- and submicrometer-sized beads, this linear range coincides with the trapping region in free solution.

In this letter, we address the advancing approach to measure local interactions by using subwavelength-sized (sub-\( \lambda \)) nonspherical particles as local probes (Fig. 1). It is known that dielectric elongated (e.g., cylindrical) objects are trapped with their long axis along the optical axis. Random thermal forces induce fluctuations not only in the particle’s position but also in its orientation: A cylindrical particle scans its local environment with three positional and two orientational degrees of freedom. We sketch possible applications utilizing this behavior: First, elongated probes in surface scanning microscopy (Fig. 1) produce a much sharper tip compared to spherical probes of the same volume. Second, it is possible to determine the force exerted by a trapped elongated bacterium just by measuring its axial displacements in the trap. Third, elongated probes can be applied to study torsion and torques of single biomolecules like rotary motors or DNA (Fig. 1). In order to use elongated probes, it is crucial to measure both the probe’s position and orientation. Furthermore, the interaction of optical and random thermal forces can play a key role for the alignment of sub-\( \lambda \) particles in nanotechnology.

Elongated particles have been used in optical trap based scanning force microscopy, but no discrimination has been made between positional and orientational contributions to the detection signal. Furthermore, a thorough theoretical study has investigated optical trapping forces and torques on cylindrical particles based on an enhanced ray-optics model that does not cover sub-\( \lambda \) particles. There has been little theoretical wave-optical analysis of the position and orientation detection of sub-\( \lambda \) nonspherical particles in highly focused fields.

The position and orientation of a cylindrical object is characterized by five parameters. Obviously, if these are independent they cannot be determined simultaneously by the four QPD signals. Nevertheless, we will suggest a method to extract orientational information from the three position signals.

The scattering of light by small arbitrarily shaped particles in highly focused fields can be described by the Rayleigh–Gans (RG) scattering theory in combination with...
Fourier-optical methods, the focused field is decomposed into plane waves. The angular spectrum of the field can be described by a generalized aperture function. A single plane wave (index $i$) from the incident spectrum has a propagation direction described by the wave vector $k$ and a linear polarization along the unit vector $\hat{p}_i$. The angular spectrum is limited by $(k_{\text{OL}}^2+k_{\text{i}}^2)^{1/2}<2\pi NA/\lambda$, where $NA$ is the numerical aperture of the OL. If the phase shift induced by the laser power, cause a Gaussian-shaped trap of the OL. If the phase shift induced by the spherical probe is tilted by $u$, the phase shift is $k\cdot x\hat{u}$. The position is therefore proportional to $\langle x(r) \rangle$, where $x(r)$ is the position of the spherical particle. The phase shift is $k\cdot x\hat{u}$.

The form factor is the Fourier transform of the particle’s shape function, which is defined to be 1 inside the particle and 0 outside. In case of a cylindrical particle with height $h$ and radius $r$, the form factor is $F(k) = \frac{\sin(hk/2)}{hk/2} J_1(rk)$, where $k = \sqrt{k_x^2+k_y^2+k_z^2}$.

In the case of the spherical particle, the position signals are to a fairly good approximation orthogonal and linear in the trapping region. However, for larger displacements of the particle, the signals (in particular the $z$ signal) become distorted. The position signals for a cylindrical probe are weaker (Fig. 3, top), but have far better orthogonality and linearity. Note the different scaling for the spherical (top graph, left axis) and the cylindrical particle (right axis). The detector sensitivity in the axial direction ($dS_z/dz$) is decreased by a factor of ~60 for the cylindrical particle compared to the spherical particle, and in the lateral $x$ direction the factor is ~30 (no linescan shown).

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If the cylinder is tilted compared to the optical axis ($\theta \neq 0^\circ$), the position signal grid is sheared (Fig. 2, right). If $F(k) = \frac{\sin(hk/2)}{hk/2} J_1(rk)$, where $k = \sqrt{k_x^2+k_y^2+k_z^2}$.

FIG. 2. Position signals $S_x$ and $S_z$ as a function of the particle position. Left: $S_x(x,0,z)$ (solid contour lines) and $S_z(x,0,z)$ (dashed contour lines) for a spherical particle. Middle: For a cylindrical particle aligned along the optical axis. Right: For a tilted cylindrical particle.
the cylinder is tilted in the $xz$ plane ($\phi=0^\circ$), the $S_x$ and the $S_z$ signals are coupled. For a tilting in the $yz$ plane ($\phi=90^\circ$), the $S_y$ and $S_z$ signals are decoupled and the $S_x$ and $S_z$ signals are coupled (not shown). In the case of a cylinder that is long compared to the focal spot, the coupling behavior can be explained by simple geometrical considerations. In common optical trapping experiments with a QPD particle tracking system, a linear and orthogonal dependency $S_j = \lambda_j \delta x_j$ between the particle position $\delta x_j$ and the corresponding signal $S_j$ is assumed. However, as we see in the right-hand part of Fig. 2 for a cylindrical probe, a more suitable approximation is $S_j = \sum_{k=x,y,z} \lambda_{jk} k$. The coupling between the lateral displacement in the $x$ direction and the $S_x$ signal, i.e., the factor $\lambda_{xz} = dS_z/dx$, is in the tilting range $0^\circ-30^\circ$ approximately linear with $\sin \theta$ (Fig. 3, bottom graph). For a tilt in the $yz$ plane, i.e., for $\phi=90^\circ$ or $270^\circ$, this coupling vanishes. As a result of geometrical considerations, the coupling between $S_x$ and the lateral signals should be minimal for $\theta=0^\circ$ and $90^\circ$. As the coupling between the signals $S_x$, $S_y$, and $S_z$ depends on the orientation of the particle, we propose an auto- and cross-correlation analysis of the signals in order to get orientational information. For example, in surface scanning microscopy, the average azimuthal angle $\phi$ of the cylinder tilted due to surface friction is determined by the scanning direction. Therefore, if the scanning is performed in the $x$ direction, the cross correlation of the $S_x$ and $S_z$ signals is approximately proportional to $\sin 2\theta$. However, there is still a need for a calibration method for the orientation measurement.

Although position signals for a cylinder that is perfectly aligned along the optical axis show a better linearity and orthogonality than signals for a comparable sphere, thermal fluctuations in the cylinder orientation lead to a decrease in the accuracy of position reconstruction. The restoring torque is to a good approximation proportional to $\theta$ in the range $0^\circ-30^\circ$. Therefore, the probability of finding the cylinder in a certain orientation is Gaussian shaped in $\theta$ with a width $\sigma_\theta$.

The calibration for spheres can be facilitated by thermal noise analysis, assuming $S_j = \lambda_j \delta x_j$. Using a cylindrical probe, one can analyze the particle fluctuations in the same manner, i.e., ignoring the coupling factors $\lambda_{xy}$, $\lambda_{xz}$, etc. Of course, due to the orientational fluctuations, this method leads to errors $\Delta j_x = j_x - S_j / \lambda_j$ in the determination of the cylinder position. The standard deviations $\sigma_{\Delta x}$ of these errors increase with increasing orientational fluctuations (Fig. 4). For a small trapping volume (Fig. 4, left-hand graph), the position detection of the cylinder in the $z$ direction is better than, and in the $x$ direction comparable to, the detection of the spherical particle if $\sigma_x < 4 \sigma_z$. In this case, the cylinder position reconstruction uncertainties are $\sigma_{\Delta x} < 2 \text{nm}$ and $\sigma_{\Delta z} < 6 \text{nm}$. If the trapping volume is increased (Fig. 4, right-hand graph), the uncertainties for the cylinder are almost unaffected, whereas the uncertainties for the sphere increase. In this case, the cylinder position detection in the $z$ direction is better than, and in the $x$ direction comparable to.

FIG. 4. Position reconstruction accuracy for a spherical and a cylindrical probe. Shown are the widths $\sigma_{\Delta x}$, $\sigma_{\Delta z}$ of the distributions of position errors $\Delta x_j$, $\Delta z_j$ as a function of the range $\sigma_\theta$ of the orientational fluctuations in $\theta$ for a small (left-hand graph) and a big (right-hand graph) trapping volume. The trapping volumes are $(\sigma_x, \sigma_y, \sigma_z) = (23, 17, 47) \text{nm}$ and $(\sigma_x, \sigma_y, \sigma_z) = (45, 35, 94) \text{nm}$, respectively.

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