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Mathematical Model of a Nanosensor Based on Optical Tweezers

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***Abstract*—The paper considers the conditions for capturing a dielectric nanoparticle in a liquid by an optical tweezers trap. It is shown that the displacement of a nanoparticle from the equilibrium position under the action of a local physical field not associated with a laser trap shaper can be used to create a nanosensor for fields of physical or chemical origin.**

***Keywords* — laser; nanosensor; force measurement; nanoparticle; optical tweezers; mathematical model.**

I. Introduction

The invention of the optical tweezers in 1969 by the American physicist A. Ashkin became the basis for developing two directions of nanotechnology – the contactless manipulation of nanoparticles and the use of nanoparticles captured by the optical trap of tweezers as nanosensors.

The manipulation of nanoparticles with optical tweezers has opened up new directions in microbiology and nanotechnology. Controlling individual biomolecules' spatial position made it possible to trace proteins' interactions with each other and with DNA [1]. Optical manipulation made it possible to sort and examine cells [2]. The ability to assemble cells into structures used to develop new drugs and counteract cancer cells has proved to be especially valuable [3].

If the manipulation of biological objects occurs mainly in liquid, then the capture of an individual particle in air opens up opportunities for a complete study of its properties since the observation time of a particle can be made longer, and it is easier to eliminate the influence of external factors on it [4].

Computer simulation of optical tweezers' interaction with nanoparticles makes it possible to assess this device and the potential areas of its application [5].

The first model of optical tweezers appeared in 1970 in the article by A. Ashkin [6]. Ashkin showed that a laser beam focused into a colloidal solution attracts the colloid's microparticles to its axis and accelerates them. In the experiments, he used radiation from an argon laser with a wavelength of λ = 514 nm and a power of P = = 19 mW, which in the focal region formed a waist (neck) of the beam with a radius of w_0 = 6.2 μ. The transparent spherical latex particles dispersed in the water had a radius of a = 1.3 μ.

The model of laser capturing the dielectric microsphere, which is much larger than the wavelength of laser radiation, was proposed by W. Wright and colleagues' article back in 1990 [7]. As in Ashkin's, the model was based on a geometric interpretation of the interaction of a laser beam with a microsphere. The model used the method for calculating the reflection and refraction of oblique rays (non-coplanar with the beam axis), described in the book by M. Born and E. Wolf [8].

In 1992, Ashkin showed that using the ray model of a laser beam's interaction with a particle (the so-called Mie scattering mode), it is possible to calculate the forces acting on a particle in a laser beam [9].

J. Harada and T. Asakura described in 1996 the effect of light on a dielectric particle much smaller than λ (the so-called Rayleigh scattering mode) [10].

The general case of optical capture of dielectric particles less than or equal to λ was described in 2001 by A. Robach and E. Stelzer [11].

In one of the first, if not the first, optical nanosensors, a nanoparticle moved with optical tweezers was associated with fluorescein, and it was determined from the shift of its fluorescence spectrum that the pH of water is different near the wall of a glass vessel and in-depth [12]. In later versions of optical nanosensors, in addition to fluorescence, the violation of the total internal reflection of light and the formation of an evanescent field [13, 14], localized surface plasmon resonance [15, 16], surface-enhanced Raman light scattering [17, 18], and optical-mechanical phenomena [19, 20] began to use.

Particles used in the nanosensors range in size from 1 to 100 nm. The particle material (metal, semiconductor, or dielectric) determined the nature of the interaction with laser radiation and measured quantities.

The article describes a mathematical model of an optomechanical nanosensor based on optical tweezers with a dielectric nanoparticle as a probe.

II. Equilibrium conditions of a dielectric particle in the optical trap

Let us consider the conditions for capturing a spherical dielectric particle by a waist of a Gaussian laser beam with a wavelength λ and power P. Let the particle

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immersed in a liquid with a refractive index n0 has a refractive index n and a radius $a << \lambda$.

Assume that the center of the waist of the laser beam (optical trap of the tweezers) coincides with the origin of the Cartesian coordinate system XYZ, the laser beam is directed vertically downward along the Z-axis, and (x_A, y_A, z_A) are the coordinates of the particle at the point A (Fig. 1).

In a liquid, an illuminated particle is influenced by five forces – gravity F_g, Archimedes force F_{Ar}, scattering force F_{scat},, and gradient force F_{grad} created by the laser beam, and the Stokes force F_{St} (friction force appearing when the particle moves). Let F be the resultant of these forces, then its components along the X, Y, and Z axes can be represented as

$$F_x = \pm F_{scat.x} \pm F_{grad.x} - F_{St.x}\,, \tag{1}$$

$$F_y = \pm F_{scat.y} \pm F_{grad.y} - F_{St.y}\,, \tag{2}$$

$$F_z = F_{scat.z} - F_{Ar} + F_g \pm F_{grad.z} - F_{St.z}\,, \tag{3}$$

where in formulas (1), (2), and (3) the sign "+" corresponds to the conditions $x - x_0 < 0$, $y - y_0 < 0$, $z - z_0 < 0$.

The resultant force of gravity and the force of Archimedes can be found by the formula

$$F_g - F_{Ar} = \frac{4}{3}\pi a^3 \left(\rho - \rho_0\right) g\,, \tag{4}$$

where ρ is the density of the particle, ρ_0 is the density of the liquid, g is the strength of the gravitational field.

The scattering force can be represented as [21]

$$\mathbf{F}_{scat} = \frac{8}{3}\pi k^4 a^6 \frac{n_0}{c}\left(\frac{n^2 - n_0^2}{n^2 + 2n_0^2}\right)^2 \mathbf{S}\,, \tag{5}$$

where k is the wavenumber ($k = 2\pi/\lambda$), c is the speed of light in vacuum, **S** is the Poynting vector.

The Poynting vector is directed along the axis of the laser beam Z only at the beam waist. Outside the waist, at some point $A(y_A, z_A)$ of the axial section of the beam, it coincides with the tangent to the hyperbolic generatrix of the beam drawn at this point. The shape of the hyperbola is determined by the numerical aperture of the focusing lens of the optical tweezers $NA = n_0 \sin\theta$, where θ is half of the angular aperture of the lens; the angle:

$$\theta = \arcsin\left(\frac{NA}{n_0}\right) \tag{6}$$

set the slope of the AO asymptote of the beam's hyperbolic generatrix relative to the beam axis Z.

Let us write the equation of the hyperbola (according to the notation in Fig. 1) in the canonical form:

$$\frac{y^2}{p^2} - \frac{z^2}{q^2} = 1\,, \tag{7}$$

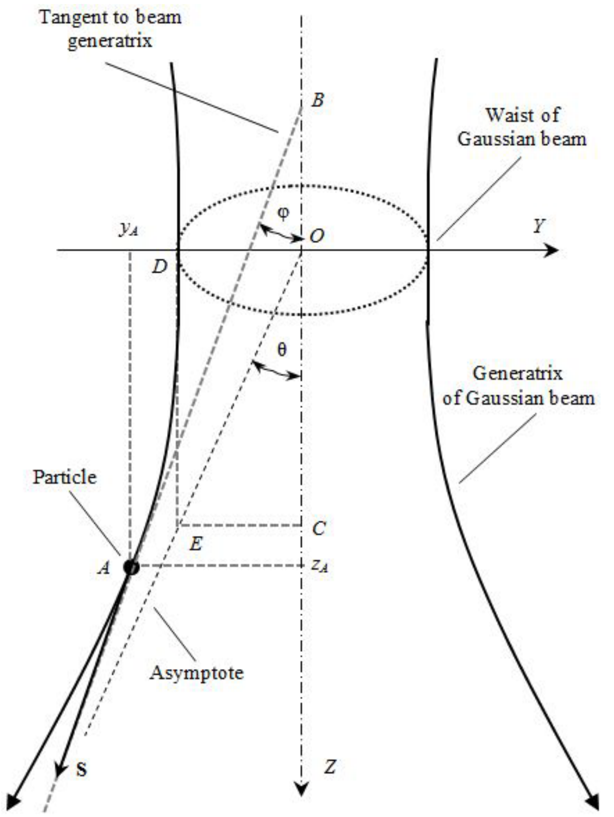

Fig. 1 Relationship of geometric parameters of a laser beam with the direction of the Poynting vector **S**

where $p = DO = w_0$ and $q = CE / \tan\theta = DO / \tan\theta = w_0 / \tan\theta$.

Substituting these parameters of the hyperbola, as well as the relation (6) into equation (7), we obtain

$$y = \left(w_0^2 + z^2 \tan^2 \arcsin\frac{NA}{n_0}\right)^{1/2}.$$

The direction of the scattering force vector F_{scat} coincides with the direction of the Poynting vector **S**. If the point A, in which the particle is located, lies on the hyperbolic generatrix of the beam, then the Poynting vector lies on the tangent drawn to the hyperbola at this point. The angle of inclination of this tangent can be found by taking the derivative of the function $y(z)$ at point A:

$$\tan\varphi = \frac{dy}{dz}\bigg|_{z=z_A} = \frac{z_A \tan^2 \arcsin\left(NA/n_0\right)}{\left[w_0^2 + z_A^2 \tan^2 \arcsin\left(NA/n_0\right)\right]^{1/2}}.$$

Note that all the calculations and constructions presented below concern only particles located on the axis or the hyperbolic generatrix of the beam, the shape of which is known and it is known where the Poynting vector is directed on this generator.

Let us replace the vectors in formula (5) by their moduli and take into account that the modulus of the Poynting vector can be approximately represented by the intensity I of the laser beam:

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$$\left|\mathbf{F}_{scat}\right| = K_1 \frac{n_0 a^6 I}{c\lambda^4}\left(\frac{n^2 - n_0^2}{n^2 + 2n_0^2}\right)^2, \quad (8)$$

where $K_1 = 1{,}31 \cdot 10^4$.

In the case of a Gaussian laser beam profile, the radiation intensity

$$I \equiv I(x,y,z) = I_0 \left[\frac{w_0}{w(z)}\right]^2 \exp\left[-\frac{2\left(x^2+y^2\right)}{w^2(z)}\right], \quad (9)$$

where for a waist radius w_0, the axial beam intensity is

$$I_0 = \frac{2P}{\pi w_0^2}, \quad (10)$$

and the beam radius at a distance z from the waist is

$$w(z) = \left(w_0^2 + z^2 \tan^2 \arcsin\frac{NA}{n_0}\right)^{1/2}. \quad (11)$$

Taking into account formulas (9), (10), and (11), the intensity distribution in the cross-section of a Gaussian beam can be written as

$$I(x,y,z) = \frac{2P}{\pi w^2(z)} \exp\left[-\frac{2\left(x^2+y^2\right)}{w^2(z)}\right]. \quad (12)$$

Substituting formula (12) into formula (8), we find the value of the modulus of the scattering force vector for an arbitrary point of the Gaussian beam:

$$\left|\mathbf{F}_{scat}\right| = K_1 \frac{2n_0 a^6 P}{c\lambda^4 \pi w^2(z)}\left(\frac{n^2 - n_0^2}{n^2 + 2n_0^2}\right)^2 \cdot \exp\left[-\frac{2\left(x^2+y^2\right)}{w^2(z)}\right]. \quad (13)$$

From the above ratios, the modulus of the scattering force vector can be determined only for points located on the hyperbolic guide and on the beam axis.

According to formula (13), the axial scattering force is

$$F_{scat}(z) = K_1 \frac{2n_0 a^6 P}{c\lambda^4 \pi w^2(z)}\left(\frac{n^2 - n_0^2}{n^2 + 2n_0^2}\right)^2. \quad (14)$$

The gradient force is described by the formula [21]:

$$\mathbf{F}_{grad} = \frac{16\pi a^3 n_0}{c}\left(\frac{n^2 - n_0^2}{n^2 + 2n_0^2}\right)\nabla\left|\mathbf{S}\right|, \quad (15)$$

where $\nabla|\mathbf{S}|$ is the gradient of the Poynting vector modulus, which can be represented by the radiation intensity gradient ∇I. A dielectric particle in the field of action of the beam is pulled onto the axis if $n > n_0$, and is expelled from the beam if $n < n_0$.

The axial gradient force is described by the formula

$$F_{grad}(z) = -\frac{64\pi^2 w_0^2 a^3 n_0 \lambda^2 P z}{c\left(\pi^2 w_0^4 + \lambda^2 z^2\right)^2}\left(\frac{n^2 - n_0^2}{n^2 + 2n_0^2}\right). \quad (16)$$

Let us find the ratio of the forces acting in the center of the laser beam waist. For this, we take the following values of the model parameters:

- ambient temperature $T = 293$ K;
- wavelength of laser radiation $\lambda = 520$ nm;
- power of laser radiation $P = 100$ mW;
- radius of the laser beam waist $w_0 = 1$ μ;
- the numerical aperture of the objective $NA = 0.95$;
- refractive index of liquid (water) $n_0 = 1.33$;
- liquid density $\rho_0 = 1000$ kg/m^3;
- particle radius $a = 10$ nm;
- the density of the particle material (titanium dioxide, TiO_2) $\rho = 4050$ kg/m^3;
- – refractive index of the particle material $n = 2.3$.

According to formulas (12), (13), and (14), the scattering force

$$F_{scat0} = \frac{2K_1 n_0 a^6 P}{c\lambda^4 \pi w_0^2} = 5{,}05 \cdot 10^{-17}\ \text{N},$$

according to formulas (15) and (16), the gradient force $F_{grad0} = 0$, and the difference between gravitational and Archimedean forces

$$F_g - F_{Ar} = \frac{4}{3}\pi a^3 \left(\rho - \rho_0\right) g = 1{,}25 \cdot 10^{-19}\ \text{N}.$$

In the further analysis, the last two forces can be neglected.

Using the formula (11), we obtain the dependence of the axial scattering force on the distance to the center of the waist (Fig. 2). Using the formula (16), we derive a similar dependence for the gradient force (Fig. 3).

As expected, at the center of the waist, the laser beam's intensity is maximum, and the scattering force takes on a maximum value, and the gradient force disappears but increases very rapidly with distance from the center. To investigate the waist region, let us plot the dependencies $F_{scat}(z)$, $F_{grad}(z)$ and $F(z) = F_{scat}(z) + F_{grad}(z)$ on one graph. From the graphs shown in Fig. 4, it can be seen that the scattering and gradient forces balance each other at the axial point with the coordinate z_{eq0} = 17 nm. This point is the center of the optical trap for a dielectric particle in the considered model of optical tweezers.

Note that in a parallel Gaussian beam, the gradient force is present only at the off-axis points of the beam, and after the particle is attracted to the axis, only the scattering force acts on the particle.

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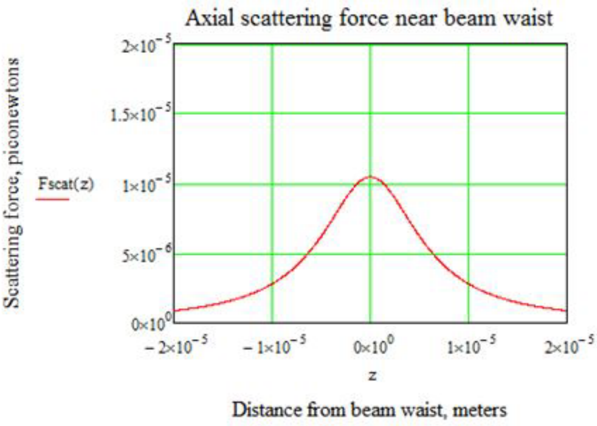

Fig. 2 Dependence of the axial scattering force on the distance before the waist of the Gaussian laser beam waist

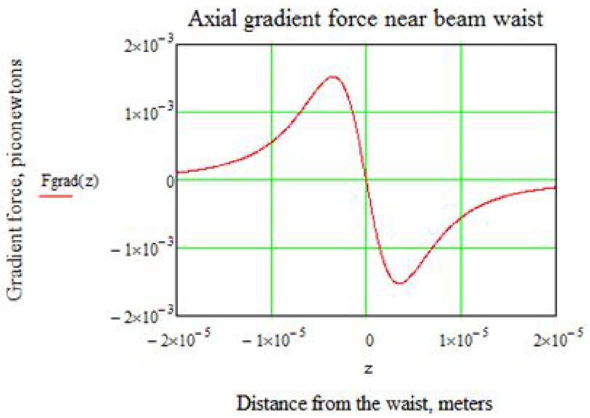

Fig. 3 Dependence of the axial gradient force on the distance to the center of the laser beam waist

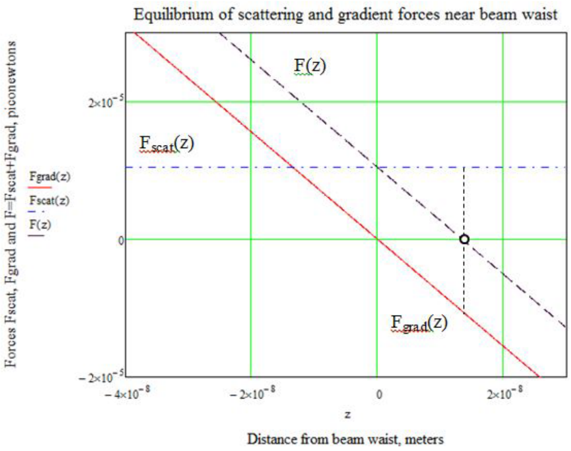

Fig. 4 Equilibrium of the scattering and gradient forces near the center of the waist Gaussian laser beam (the equilibrium point z_0 is marked with circle)

III. Optical Tweezers as a Sensor

Let us consider what additional forces can move the particle from the equilibrium position. If a particle is near the surface of a solid, surface forces begin to act on it. At a distance $L < 100$ nm, interaction forces appear between the particle and the body surface, usually invisible at a greater distance. The nature of such interaction may be:

- electrostatic;
- magnetic;
- intermolecular (van der Waals force);
- hydrophobic;
- hydrogen bonding.

The last two types of interactions are chemical and appear at a distance of $L < 1$ nm. We will not consider them but dwell on a more long-range force – the van der Waals force.

Additional force F_{ad} appeared in the laser beam waist leads to a displacement of the particle from the equilibrium position with the z_0 coordinate to the place with the z_1 coordinate. If an additional force acts along the Z-axis, then the particle's equilibrium occurs under condition $F_z + F_{ad} = 0$. The magnitude of the displacement $\Delta z = z_1 - z_0$ is a characteristic of this force. We can also assume that $w(z) = w_0$ because the particle is in an optical trap. Near the equilibrium point, the Stokes force becomes negligible. Then, in the presence of additional force, the equilibrium according to formulas (3), (4), (14), and (16) is determined by the equation

$$K_1 \frac{n_0 a^3 P}{c\lambda^4 \pi w_0^2}\left(\frac{n^2 - n_0^2}{n^2 + 2n_0^2}\right)^2 - \\ -\frac{32 n_0 \lambda^2 P z_1}{c\pi^2 w_0^6}\left(\frac{n^2 - n_0^2}{n^2 + 2n_0^2}\right) + F_{add} = 0. \tag{17}$$

Equation (17) can be considered as a mathematical model of this nanosensor used as a force meter. This equation takes into account that near the equilibrium position $\pi^2 w_0^4 >> \lambda^2 z_1^2$.

If a nanoparticle of radius a approaches the flat surface of a solid at a distance $L << \lambda$, then the van der Waals force begins to act on it [17]:

$$F_{VdW} = \frac{C_H a}{6L^2}\ , \tag{18}$$

where C_H is the Hamaker constant, which for most solids is in the range of 10^{-19}–10^{-20} J. Taking $C_H = 10^{-20}$ J, we find the dependence of this force on the distance for particle radius values of 10, 50, and 100 nm (Fig. 5).

As shown in [22], the lower threshold for measuring force using optical tweezers is approximately 1 fN. Fig. 5 shows that at a distance of 100 nm from the surface, even the smallest of the considered particles – a particle with a radius of 10 nm – is acted upon by force greater than 1 fN. Note that such a particle's movement along the surface, which can be realized using a two-coordinate stage with a piezo drive, makes it possible to measure the surface nanorelief.

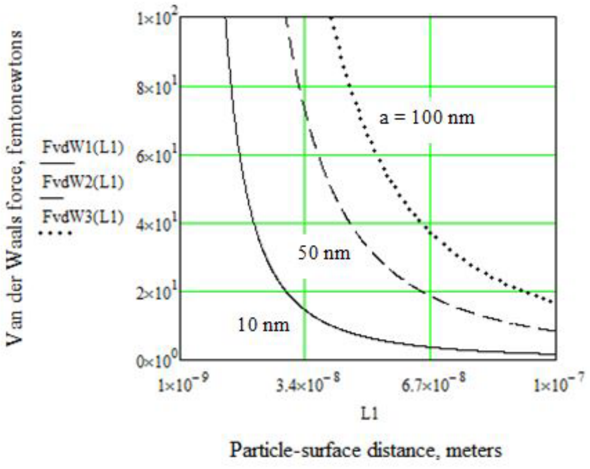

Fig. 5 Dependence of the van der Waals force on distance of a particle to the surface of a solid for three values of the particle radius

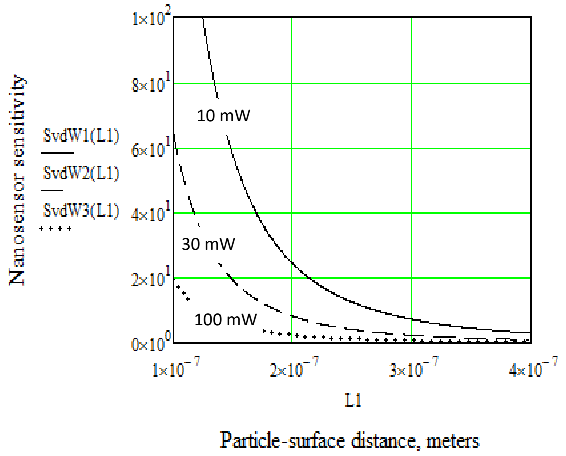

Fig. 6 Dependence of nanosensor sensitivity to a displacement of the surface of a solid in the zone of action of the van der Waals force

Let us assume that the surface of a solid body is perpendicular to the Z-axis, and the particle is brought closer to this surface, which is in an optical trap in a state of equilibrium. Taking into account the action of the van der Waals force (18), the equilibrium condition (17) takes the form:

$$K_1 \frac{n_0 a^3 P}{c\lambda^4 \pi w_0^2}\left(\frac{n^2-n_0^2}{n^2+2n_0^2}\right)^2 - \frac{32 n_0 \lambda^2 P z_1}{c\pi^2 w_0^6}\left(\frac{n^2-n_0^2}{n^2+2n_0^2}\right)+\frac{C_H a}{6L^2}=0.$$

The sensitivity of a sensor based on optical tweezers and a dielectric nanoparticle to the van der Waals force is determined by the ratio:

$$S_{VdW}=\frac{dz}{dL}=-\frac{cC_H\left(n^2+2n_0^2\right)aw_0^2}{96\left(n^2-n_0^2\right)n_0\lambda^2 PL^3}.$$

Fig. 6 shows the dependence $S_{VdW}(L)$ for a particle with a radius of a = 10 nm and three values of the laser radiation power. The S_{vdW} sensitivity shows how many times the axial displacement of a particle under the van der Waals force's action is greater than the displacement of the surface in the opposite direction. For example, if, at a radiation power of P = 30 mW, the surface located at a distance of L = 100 nm is displaced by a value of ΔL = = 1 nm, then the particle moves towards the surface at a distance of Δz = 65 nm. Thus, optical tweezers with a nanoparticle in an optical trap can be used as a sensitive sensor for ultra-low forces of various origins that violate the initial equilibrium of the nanoparticle.

IV. Influence of Brownian Motion on the Accuracy of Particle Positioning

A nanoparticle in a liquid moves chaotically under the impact of molecules of the medium (Brownian motion). In the XY plane, perpendicular to the Z-axis of the laser beam, for a time interval Δt, a spherical particle of radius a moves according to the Stokes-Einstein equation at a distance with an RMS value

$$\langle \Delta r\rangle=\sqrt{\frac{2k_B T\Delta t}{3\pi\eta a}},$$

where k_B is the Boltzmann constant, T is the temperature of the liquid, η is its viscosity. Due to the Brownian motion, a particle with a radius of 10 nm, which is in water with a temperature of 293 K, will move by an average of 1 μ in 10 ms if it is no force will act. If the particle is in the laser beam's gradient electric field, the particle's random motion will be suppressed the stronger, the greater the power of the laser beam and the sharper its focusing.

In the laser beam's waist, the particle falls into the potential well created by the gradient force. The Brownian motion of a particle near the waist can be neglected if the depth of the potential well is much greater than the kinetic energy of the particle's Brownian motion. This condition can be written as [21]

$$\frac{n\left(n^2-n_0^2\right)a^3 P}{cn_0\left(n^2+2n_0^2\right)w_0^2}\ge 3k_B T. \qquad (19)$$

To fulfill condition (19) at n = 2.3, n_0 = 1.33 and T = = 293 K, the laser radiation power (in watts) must be related to the particle radius (in meters) by the ratio $P \ge 1{,}3\cdot 10^{-24} a^3$. For a = 10 nm, a power P = 1.3 W is required, and for 100 nm – 1.3 mW.

Conclusions

Based on an analysis of the forces acting on a dielectric nanoparticle near the waist of a Gaussian laser beam, a mathematical model of optical tweezers is constructed, and the formation of an optical trap capable of capturing a particle and holding it in the waist is demonstrated. Calculations have shown that in a focused laser beam, the gradient force prevails over the scattering force and is equalized to it only in the focus's immediate vicinity. Equilibrium conditions for a nanoparticle in a focused laser beam are found.

The influence of the Brownian motion of the molecules of the medium (water) on the nanoparticle's

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positioning accuracy is considered. It has been established that a particle with a radius of 10 nm, which is in water, in 10ms can be at a distance of 1 μ from its initial position if no forces act on it. If the power of the laser radiation is sufficient for the depth of the potential well created by the gradient force to significantly exceed the kinetic energy of the Brownian motion of the particle, then the effect of the latter on the particle positioning accuracy can be neglected.

It is confirmed that the motion of a particle in a medium with nonzero viscosity occurs at a constant speed and depends on the radius of the particle and the radiation intensity within the particle cross-section. The value of the particle velocity, obtained from the developed mathematical model of the optical tweezers, coincides with high accuracy with the value found by Ashkin [6].

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Математична модель наносенсора на основі оптичного пінцета

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***Анотація*—Стаття присвячена оптичному пінцету – пристрою, який дозволяє безконтактно маніпулювати частинками мікронних та субмікронних розмірів. Ця властивість оптичного пінцета вже понад тридцять років використовується в мікробіології і дає змогу сортирувати клітини та досліджувати взаємодію протеїнів між собою та з ДНК. У статті розглянуто сили, які виникають в перетяжці сфокусованого лазерного пучка і які дають змогу створити оптичну пастку для частинки.**

З боку лазерного пучка діють розсіювальна сила (тиск світла) та градієнтна сила електричного поля світлової хвилі. З боку середовища на частинку також діють сила тяжіння та сила Архімеда. Рух частинки в рідині або повітрі викликає появу сили опору середовища – сили Стокса. У разі відсутності градієнтної сили сила Стокса стабілізує швидкість частинки через деякий час після початку дії на неї тиску світла або зовнішнього електричного поля. У роботі показано, що в фокальній області сфокусованого лазерного пучка градієнтна сила значно переважає розсіювальну силу і вони зрівнюються тільки у точці рівноваги частинки, розташованій поблизу фокуса.

У статті проаналізовано умови захоплення діелектричної наночастинки пасткою оптичного пінцета та вплив на положення частинки локальних електричних полів. Частинка, захоплена пасткою, знаходиться на осі лазерного пучка, на невеликій відстані від перетяжки.

Якщо локальне електричне поле прикладається вздовж осі лазерного пучка, то частинка переходить в нове положення рівноваги. За величиною осьового зміщення частинки можна оцінити напруженість поля. Локальне електричне поле виникає, наприклад, у разі міжмолекулярної взаємодії і появи ван дер Ваальсової сили.

У роботі запропоновано використовувати оптичний пінцет з наночастинкою, захопленою перетяжкою лазерного пучка, в якості наносенсора локального електричного поля. Розраховано чутливість такого наносенсора у разі дії на частинку ван дер Ваальсової сили. Запропоновано використовувати наносенсор разом з 2-координатним п'єзоприводом для зчитування нанорельєфу поверхні.

Оскільки точність запропонованого наносенсора визначається величиною похибки у вимірюванні лінійного зміщення частинки під дією локального електричного поля, то важливу роль відіграє броунівський рух частинки під дією поштовхів з боку молекул середовища. Показано, що у воді за відсутності будь-яких зовнішніх впливів частинка радіусом 10 нм за 10 мс може опинитися на відстані 1 мкм від початкового положення. Щоб запобігти такому блуканню частинки, потрібно створити для неї потенціальну яму, глибина якої більша за кінетичну енергію частинки. Знайдено умову, за якої така ситуація можлива.

Ключові слова — лазер; оптичний пінцет; оптична пастка; діелектрична наночастинка; наносенсор; чутливість; математична модель.