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Numerical study of optical trapping properties of nanoparticle on metallic film with periodic structure*

Cheng-Xian Ge(葛城昱)[1], Zhen-Sen Wu(吴振森)[1,†], Jing Bai(白靖)[1], and Lei Gong(巩蕾)[2]

[1] *School of Physics and Optoelectronic Engineering, Xidian University, Xi'an* 710071, *China*
[2] *School of Photoelectric Engineering, Xi'an Technological University, Xi'an* 710021, *China*

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Based on the three-dimensional dispersive finite difference time domain method and Maxwell stress tensor equation, the optical trapping properties of nanoparticle placed on the gold film with periodic circular holes are investigated numerically. Surface plasmon polaritons are excited on the metal-dielectric interface, with particular emphasis on the crucial role in tailoring the optical force acting on a nearby nanoparticle. Utilizing a first order corrected electromagnetic field components for a fundamental Gaussian beam, the incident beam is added into the calculation model of the proposed method. To obtain the detailed trapping properties of nanoparticle, the selected calculations on the effects of beam waist radius, sizes of nanoparticle and circular holes, distance between incident Gaussian beam and gold film, material of nanoparticle and polarization angles of incident wave are analyzed in detail to demonstrate that the optical-trapping force can be explained as a virtual spring which has a restoring force to perform positive and negative forces as a nanoparticle moves closer to or away from the centers of circular holes. The results of optical trapping properties of nanoparticle in the vicinity of the gold film could provide guidelines for further research on the optical system design and manipulation of arbitrary composite nanoparticles.

Keywords: surface plasmon, periodic circular holes, optical trapping force, Maxwell stress tensor, gold film

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1. Introduction

Since the Ashkin *et al.*'s pioneering work on trapping a dielectric microsphere by using a single focused laser beam,[5] optical trapping and manipulation of particles have been widely used in different areas of science, particularly in research of the optical trapping properties of surface plasmon polaritons (SPPs) due to their advantages of high precision and sensitivity,[1–4] It has recently been used to manipulate nanoparticle near the gold film with periodic structure. Due to their noninvasive and noncontact advantages, the significant phenomenon of surface plasmon polaritons (SPPs) have been widely used in various areas of science,[6,7] such as plasmonic optical tweezers toward molecular manipulation[8] and surface plasmon radiation forces.[9] The SPP refers to evanescent surface electromagnetic excitation that occurs on metal-dielectric interface[10,11] and have an ability to significantly improve the interaction between light and target at controlled resonance wavelength, which means that the optical trapping force acting on a nanoparticle in the vicinity of periodic structure gold film can be remarkably amplified[12] compared with the optical tweezer's optical trapping force acting on trapping and manipulating nanoparticles.[13–20] Accurate prediction of optical trapping force exerted on nanoparticles placed on the gold film which can excite SPPs induced by the illumination of Gaussian laser beam enables a better understanding of the physical mechanism of light–matter interaction, and may offer important applications in contact-free manipulation of nanoparticles. However, the investigation of optical trapping properties induced by periodic structure is rarely performed, which requires more effective methods to investigate the optical trapping properties of nanoparticle near the complex structures accurately and reliably.

Surface plasmon polaritons play a crucial role in tailoring the optical force acting on a nearby nanoparticle, which means that the optical trapping force can be tailored by changing the structure of the gold film under different conditions. This in turn enabled us to study the new aspects of specific applications[21–23] and investigate the interaction between surface plasmon polaritons and complex structure. Over the past few years, considerable research effort has focused on the optical trapping properties of particle in the vicinity of an optical surface. The lateral optical force properties of chiral particles and circularly polarizable particles next to a surface were, respectively, studied with an illumination of plane wave by Wang and Chan[24] and Rodríguez-Fortuño *et al.*[25] Beside, Petrov *et al.* found that the optical pulling force can be as-

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†Corresponding author. E-mail: wuzhs@mail.xidian.edu.cn

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sisted by SPPs for a nearby particle.[26] Shalin and Sukhov utilized plasmonic amplification for accelerating and trapping the nanoscale particles.[27] Righini *et al.* investigated the parallel and selective trapping properties in a patterned plasmonic landscape.[28] In addition, the optical trapping force properties of a nanoparticle in the vicinity of the metallic substrate with an illumination of Gaussian beam were studied by Ivinskaya *et al.*[29] Although considerable effort has been devoted to investigating the properties of optical trapping forces exerted on particle next to a surface, few studies have focusing on the nanoparticle in the vicinity of gold film with periodic structure irradiated by a Gaussian beam, especially when the gold film has periodic circular holes.

To solve the problem of achieving nanoscale localization and find the unique optical trapping properties of SPPs, plasmonic tweezers require the introduction of auxiliary structures that can excite highly confined electromagnetic fields.[30–34] The finite difference time domain (FDTD) method is a powerful and well-known technique to calculate electromagnetic fields around the nanostructures, especially when the nanostructures have complex and arbitrary geometries. According to the advantages of the finite difference time domain, this method is used to reliably analyze the electromagnetic fields when research targets are too complicated for analytical approaches.[35,36] With the development of the FDTD algorithm, once the FDTD computing model is set up accurately, it will have wide applications and become a reliable tool for investigating the properties of composite optical system. Consequently, the calculation model of nanoparticle in the vicinity of the gold film with periodic circular holes is established by using three-dimensional (3D) dispersive FDTD method. The periodic circular holes are filled with SiO_2 material. To accurately calculate the radiation pressure in arbitrary direction for the composite structure, the discrete Maxwell stress tensor is added into the calculation model by performing an appropriate conversion according to the theory of the radiation force, which is based on the foundation of theoretical analysis with taking advantage presented by many researches for the radiation pressure forces exerted on a spherical particle given by Gouesbet and Gréhan,[37] and Ren *et al.*[38,39]

In the present article, the effects of the various parameters on the composite model are investigated in detail in order to obtain the analytical results. Figure 1 shows the main schematic diagram of the present investigations. The meanings of the parameters used in our study will be discussed in detail in Section 3.

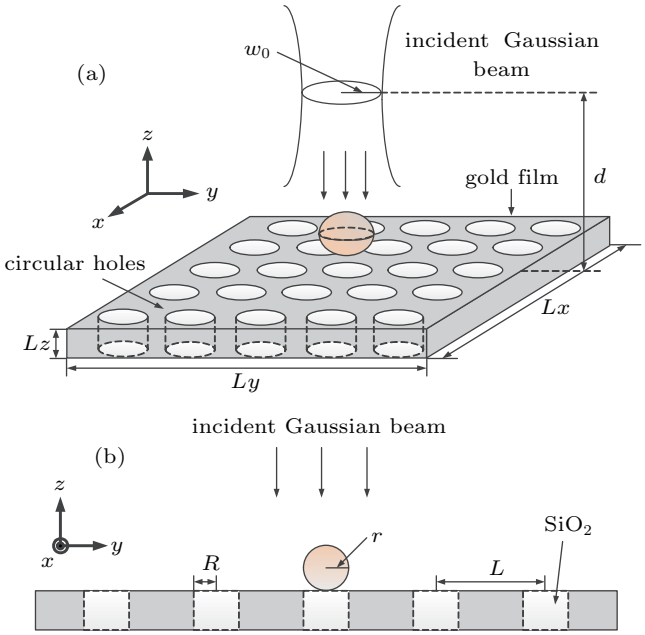


Fig. 1. Schematic diagram of spherical nanoparticle placed on gold film with periodic circular holes: (a) Full view and (b) sectional view.

2. Establishing the calculation model

2.1. Theory of Maxwell stress tensor in FDTD

To calculate the radiation pressure of nanoscale targets in near-field, we generalize the conservation law for momentum by using 3D FDTD method, which can only consider the momentum changes without taking into account the shapes of targets. In the computational field, the composite gold film and dielectric nanoparticle will reflect and refract the light, and the changes in photon momentum around the nanoparticle will induce a force exerted on this particle. As a consequence, when the electromagnetic field in the entire area of FDTD model is correctly calculated, the electromagnetic field around a nanoparticle or the other targets can be utilized to calculate the radiation pressure by using the law of momentum conservation. The conservation law of total momentum of a system can be expressed as[40]

$$\boldsymbol{F} = \int_V \boldsymbol{f}\,\mathrm{d}\tau = -\oint_S \boldsymbol{T}\cdot\hat{n}\,\mathrm{d}S. \tag{1}$$

The radiation pressure acting on the charge system in the total electromagnetic field equates the surface integral of Maxwell stress tensor $\boldsymbol{T}$ over the area S that is around the target. According to the 3D FDTD method of electromagnetic calculation, the Maxwell stress tensor $\boldsymbol{T}$ can be expressed as

$$\boldsymbol{T} = \sum_{ij}\left(\frac{\varepsilon_0\varepsilon_\mathrm{r}\boldsymbol{E}+\mu_0\mu_\mathrm{r}\boldsymbol{H}}{2}\delta_{ij} - \varepsilon_0\varepsilon_\mathrm{r}\boldsymbol{E}_i\boldsymbol{E}_j - \mu_0\mu_\mathrm{r}\boldsymbol{H}_i\boldsymbol{H}_j\right), \tag{2}$$

where $\boldsymbol{E}$ and $\boldsymbol{H}$ are respectively the vector of the electric field and magnetic field intensity in free space of FDTD model; i and j respectively represent the x, y, and z directions; δ_{ij} is the unit stress tensor; ε_0 and ε_r are respectively vacuum permittivity and relative permittivity; μ_0 and μ_r are, respectively,

vacuum permeability and relative permeability. To obtain the properties of optical trapping force exerted on a nanoparticle in the total electromagnetic field, the radiation pressure which is along each of three axial directions in a certain integral area should be calculated.[40]

By combining the above theoretical basis, the optical trapping force along the x axis can be expressed as

$$F_x = \sum_{m=a_1}^{b_1}\sum_{n=c_1}^{d_1}\left(-\frac{\varepsilon_0\varepsilon_r E_{mn}^2+\mu_0\mu_r H_{mn}^2}{2} + \varepsilon_0\varepsilon_r E_{x_{mn}}^2+\mu_0\mu_r H_{x_{mn}}^2\right)\Delta y\Delta z. \quad (3)$$

The trapping force along other two axial directions can also be obtained similarly, as follows:

$$F_y = \sum_{m=a_2}^{b_2}\sum_{n=c_2}^{d_2}\left(-\frac{\varepsilon_0\varepsilon_r E_{mn}^2+\mu_0\mu_r H_{mn}^2}{2} + \varepsilon_0\varepsilon_r E_{y_{mn}}^2+\mu_0\mu_r H_{y_{mn}}^2\right)\Delta x\Delta z, \quad (4)$$

$$F_z = \sum_{m=a_3}^{b_3}\sum_{n=c_3}^{d_3}\left(-\frac{\varepsilon_0\varepsilon_r E_{mn}^2+\mu_0\mu_r H_{mn}^2}{2} + \varepsilon_0\varepsilon_r E_{z_{mn}}^2+\mu_0\mu_r H_{z_{mn}}^2\right)\Delta x\Delta y, \quad (5)$$

where Δx, Δy, and Δz each are the 3D discrete grid space step in the calculation model of FDTD. For the convenience of FDTD calculation, a specific rectangle boundary surrounding the nanoparticle in the plane parallel to $x = 0$ plane is taken in formula (3). The $[a_1, b_1]$ and $[c_1, d_1]$ are, respectively, the projected interval in y-axis and z-axis of the rectangle boundary. The m and n in formulas (4) and (5) are the rectangle boundaries which are similar to those in formula (3).

According to this theoretical basis, the optical trapping force along arbitrary direction can be calculated by sampling the electromagnetic field on the cube boundary surrounding the nanoparticle in 3D FDTD calculation model. This is very promising as a fundamental theory to calculate the optical trapping force exerted on a nanoparticle in the near-field, which makes full use of the advantages of the FDTD method. The optical trapping force on arbitrary nanoparticle in the vicinity of the complicated structure can also be accurately calculated and investigated by using this method.

2.2. Model of full-space dispersive FDTD with Gaussian beam incidence

This paper establishes a composite model of a nanoparticle in the vicinity of the composite gold film with periodic circular holes by using 3D dispersive FDTD method with Gaussian beam incidence. A first order corrected electromagnetic field components for a fundamental Gaussian beam can be obtained from Ref. [41]. The electromagnetic field component expressions of incident Gaussian beam are suitable for FDTD iteration with appropriate conversion, which can be obtained as follows:

$$E_x = E_0\psi_0(x,y,z), \quad E_y = 0, \quad E_z = -\frac{2Qx}{l}E_x, \quad (6)$$

$$H_x = 0, \quad H_y = H_0\psi_0(x,y,z), \quad H_z = -\frac{2Qy}{l}H_y. \quad (7)$$

In the above for

$$\psi_0(x,y,z) = \mathrm{i}Q\exp\left(-\mathrm{i}Q\frac{x^2+y^2}{w_0^2}\right)\exp(\mathrm{i}kz), \quad (8)$$

where $Q = 1/(\mathrm{i}+2z/l)$, with $l = kw_0^2$ and w_0 being the beam waist radius, and k is $2\pi/\lambda$. In the 3D FDTD method, formulas (6) and (7) can be added to the connection boundary of computing space, which is different from the conventional plane wave connection boundary condition in the calculation model.

In this paper, the basic iterative framework for the 3D FDTD method is compiled based on $C++$ programming. To solve the problem of gold dispersion, the recursive convolution method of Drude dispersive medium for the FDTD analysis is used.[42,43] For the FDTD simulation, the perfectly matched layer (PML) is used as the absorbing boundary to eliminate the possible errors due to the light reflections from the outer grid boundaries. The outer grid boundaries are used to simulate the infinite space with limited space in the FDTD calculation model. The theoretical basis of the FDTD method can refer to Refs. [44]–[48]. Based on the theory of Subsection 2.1, a cube boundary surrounding the nanoparticle is used to sample and bring the value of electromagnetic field into formulas (3)–(5) for optical trapping force with arbitrary direction. To illustrate our method, figure 2 shows the primary calculation model.

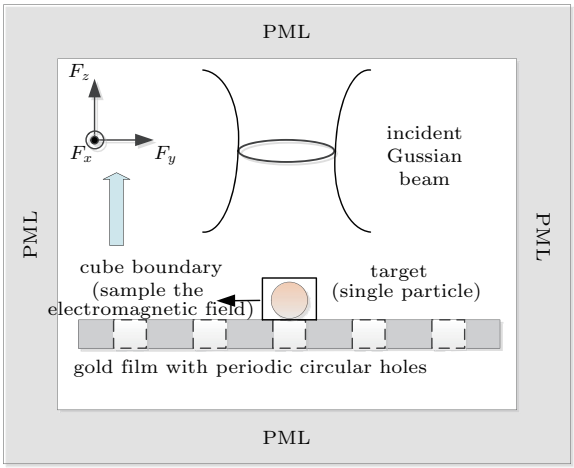


Fig. 2. Sectional view of 3D dispersive FDTD model.

3. Results of our numerical calculation

In this paper, the variable parameters of the composite structure are shown in Fig 1. Lx and Ly denote the size of the gold film; Lz represents the thickness of the gold film; w_0

is the beam waist radius of incident Gaussian beam; d is the distance between the waist center and gold film; R and r are respectively the radius of circular hole and nanoparticle. The distance between contiguous centers of circular holes can be expressed as L. For the incident Gaussian beam with linear polarization, our research focuses on the case of vertical incidence, and polarization angle of incident wave is α. The incident Gaussian beam is assumed to be symmetrically located in the central zone of gold film. The center of the structure coincides with that of the incident Gaussian beam in actual investigation. In all our calculations, the power of incident Gaussian beam going through the focal plane is $P = 100$ mW.

3.1. Numerical confirmation of the SPPs excitation

To test the calculation model and validate the accuracy of the computations, the results are selected to compare with those of different incident wavelengths provided by the same calculation model in this paper. The distribution of the magnetic field component H_z on the gold film is shown in Fig. 3 which proves the correctness of SPPs excitations. The results are obtained at different incident wavelengths ($\lambda = 0.588$ μm, $\lambda = 0.6328$ μm, $\lambda = 0.808$ μm, and $\lambda = 1.064$ μm) to prove the correctness of SPPs. For the simulation, the size of the gold film is fixed, *i.e.*, Lx and Ly are both 1048 nm, Lz is 20 nm, L and d are, respectively, 212 nm and 175 nm; radius r and the refractive index of the dielectric nanoparticle that is placed on the gold film in air are 40 nm and $(1.55, 0)$, respectively; the polarization angle of incident Gaussian beam is 0° (electric field is directed along the x axis); the radius of circular hole R is 32 nm; the beam waist radius w_0 is chosen to be 450 nm; the size of the discrete grid in the FDTD method is $\lambda/158$. The reason why these parameters are used is that they satisfy the condition of numerical dispersion stability of the FDTD method and the resonance condition of SPPs. Figure 3(b) shows that the magnetic field component H_z around the sides of circular holes along the y axis is significantly amplified by the structure of the gold film. This is the direct numerical confirmation of SPPs' excitations in the y direction. This gold film with periodic circular holes will support the SPPs' propagation. For the dielectric nanoparticle on the film, the SPPs' propagation will have a significant influence on the manipulation of this nanoparticle.

Figure 3 shows that the magnetic field component H_z on the edge of the gold film is not strong. This happens because the beam waist radius of the incident wave is limited, and the beam waist radius is smaller than the length of the gold film. Figures 3(a)–3(d) show that the distribution of the magnetic field component H_z is far less than that of the magnetic field component H_z in Fig. 3(b). Under these wavelength conditions, the structural parameters of the gold film are not sufficient for SPPs' excitation. So SPPs are excited when incident wavelength is $\lambda = 0.6328$ μm. To more clearly illustrate the excitation of SPPs, figure 4 shows the optical response of the gold film with periodic circular holes. This indicates that the scattering intensity of the composite gold film is significantly amplified when the wavelength is about $\lambda = 0.6328$ μm. Once the electromagnetic fields have been obtained by using the FDTD method, the properties of optical trapping force acting on the nanoparticle can be studied, which will be discussed in detail in Subsection 3.2.

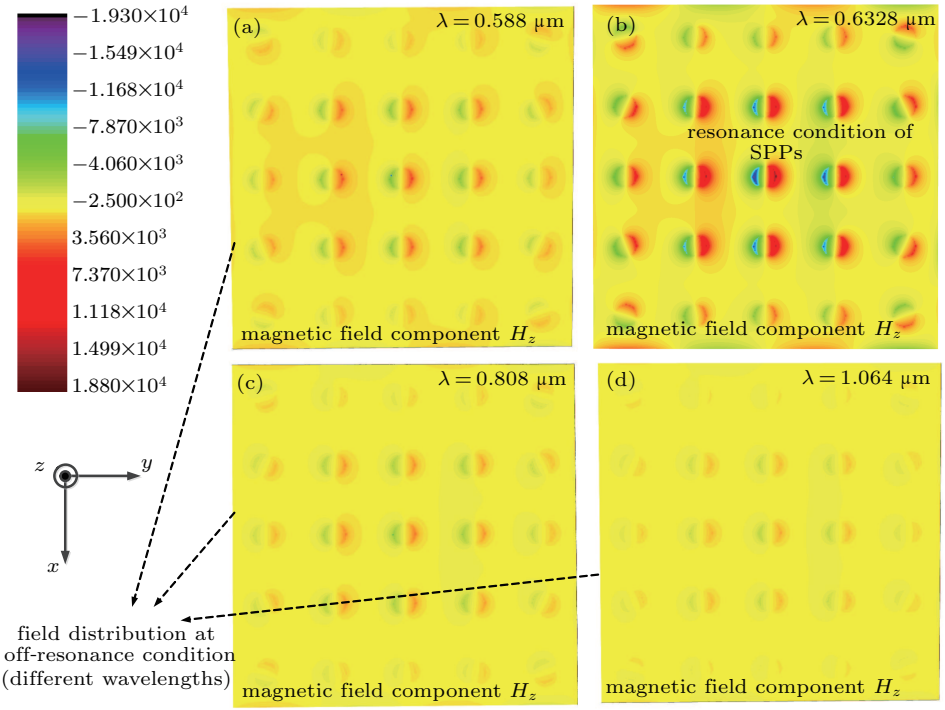


Fig. 3. Vertical view of distribution of magnetic field component H_z on the gold film for (a) $\lambda = 0.588$ μm, (b) $\lambda = 0.6328$ μm, (c) $\lambda = 0.808$ μm, and (d) $\lambda = 1.064$ μm.

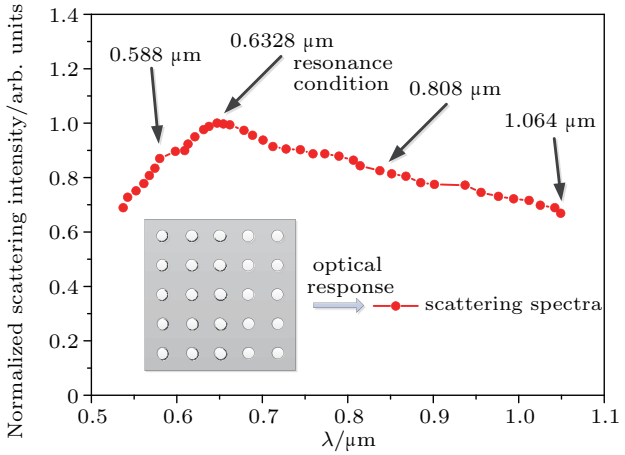


Fig. 4. Optical response of gold film with periodic circular holes.

To better illustrate the interaction and relationship between SPP and periodic structure gold film, the distribution of the magnetic field component H_z on the gold film under the resonance condition of $\lambda = 0.6328$ μm is presented in Fig. 5 using some parameters the same as those used in Fig. 3. To give readers a better understanding, the plots of vertical view and full view of SPPs on the gold film are presented in Figs. 5(a) and 5(b), respectively. Figure 5 shows that the SPPs are controlled by the periodic circular holes of gold film. The magnitude plots for the magnetic field are presented. This indicates that the electromagnetic field which occurs on the gold film around the circular holes is significantly amplified. The interaction between incident wave and the gold film with periodic circular holes causes the SPPs to change. This change is determined by the structure parameters which are connected with the radius of circular hole. This result in turn enables us to tailor the optical trapping force by changing the structure parameters of gold film, which will be discussed in detail in Subsection 3.2. In addition, the incident Gaussian beam allows us to control the circular hole that can excite the strongest SPPs. Hence, the optical film system with Gaussian beam incidence plays a crucial role in determining the overall performance.

After obtaining these results, we can investigate the optical trapping properties of nanoparticle placed on the gold film and understand the internal physical characteristics better, which means that this paper can provide a more effective method to simulate the properties of optical film system.

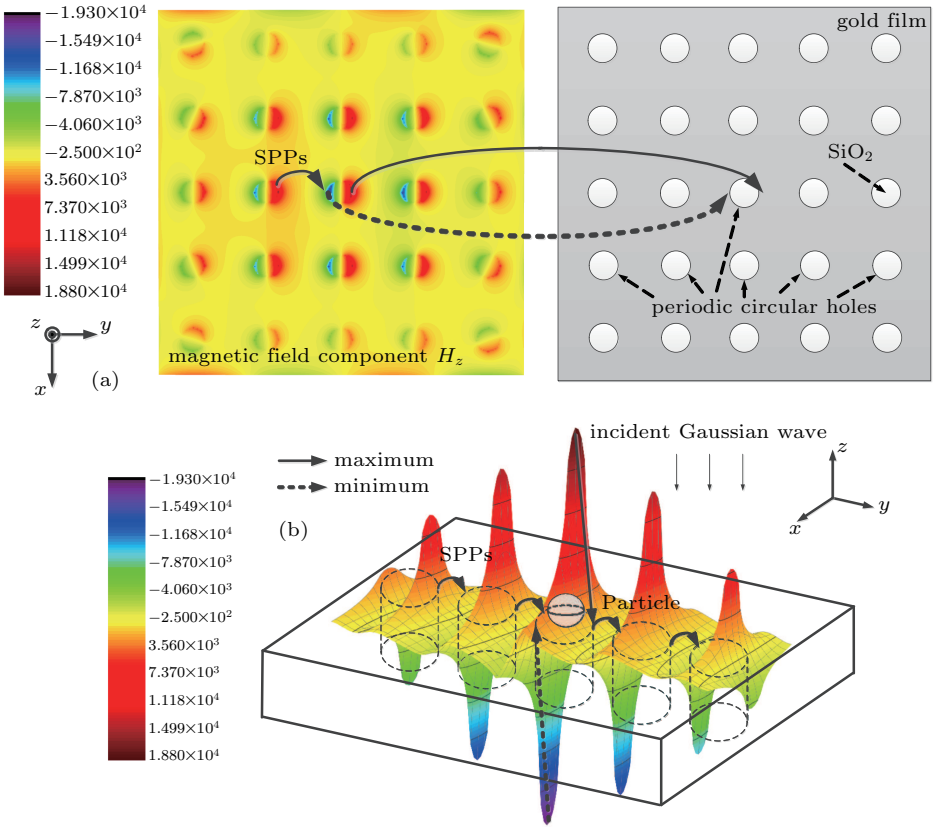


Fig. 5. (a) Vertical view and (b) full view of distribution of magnetic field component H_z on gold film.

3.2. Manipulation of nanoparticle placed on gold film with periodic circular holes

To find the properties of single nanoparticle in the vicinity of the gold film, figure 6(a) shows the optical trapping force of single nanoparticle and single nanoparticle placed on the gold film with and without periodic circular holes. The horizontal coordinate y in Fig. 6(a) is the transverse distance between nanoparticle and the incident beam. The position of nanoparticle in the x direction is $x = Lx/2$. Figure 6(b) shows the characteristic of optical trapping force exerted on nanoparti-

cle placed on the film with periodic circular holes. Due to the space symmetry of the research problem, it is clear that F_x is zero on condition that nanoparticle moves in the y direction. The trapping force F_y on condition that the nanoparticle moves in the y direction with a polarization angle of 0° will have the same properties as F_x on condition that the nanoparticle moves in the x direction with a polarization angle of 90°. The nanoparticle will be manipulated to move toward the gold film and bound on the surface, which implies that the property of lateral optical trapping force F_y in horizontal direction is more intriguing in this paper. Consequently, in this paper we mainly investigate the trapping force F_y. The incident wavelength is $\lambda = 0.6328$ μm. The beam waist radius of incident Gaussian wave is $w_0 = 250$ nm. The other parameters in Fig. 6 are the same as those used in Fig. 5.

To better investigate the manipulation of nanoparticle in the vicinity of the gold film, it is necessary to first validate the accuracy of the FDTD calculation model developed in this paper. The black dot in Fig. 6(a) represents the optical trapping force of single nanoparticle, obtained from the generalized Lorenz–Mie theory under the same parameters.[37–39] As expected, our results from the FDTD calculation model are in excellent agreement with those from the generalized Lorenz–Mie theory. This consistency can verify the validity of our theory and codes, which indicates that the accuracy of the conditions of Maxwell stress tensor and Gaussian beam in the FDTD calculation model is verified. When various conditions of FDTD method are set up and correct, this calculation model can be applied to a number of research problems, and the calculation model in this paper can be used for in-depth research in the following.

In Fig. 6(a), for the case of nanoparticle placed on the gold film without periodic circular holes, it is of interest to note that there is an opposite optical trapping force exerted on the nanoparticle compared with the scenario for the case of single nanoparticle. This indicates that the interaction between incident wave and gold film has an effect on the manipulation of nearby nanoparticle, and the gold film without periodic circular holes plays a crucial role in changing the scattering field of nanoparticle. For the case of nanoparticle placed on the film with periodic circular holes, there is a unique optical trapping force exerted on the nanoparticle. Optical trapping force is significantly larger than those in the other cases, and the optical trapping force F_y exerted on the nanoparticle is tailored by the structure of gold film, indicating that the SPPs are controlled by periodic circular holes under the illumination of Gaussian beam. To give our readers a better understanding, in Fig. 6(b) we depict the characteristic diagram of optical trapping force F_y, which is presented by the solid line with triangles in Fig. 6(a).

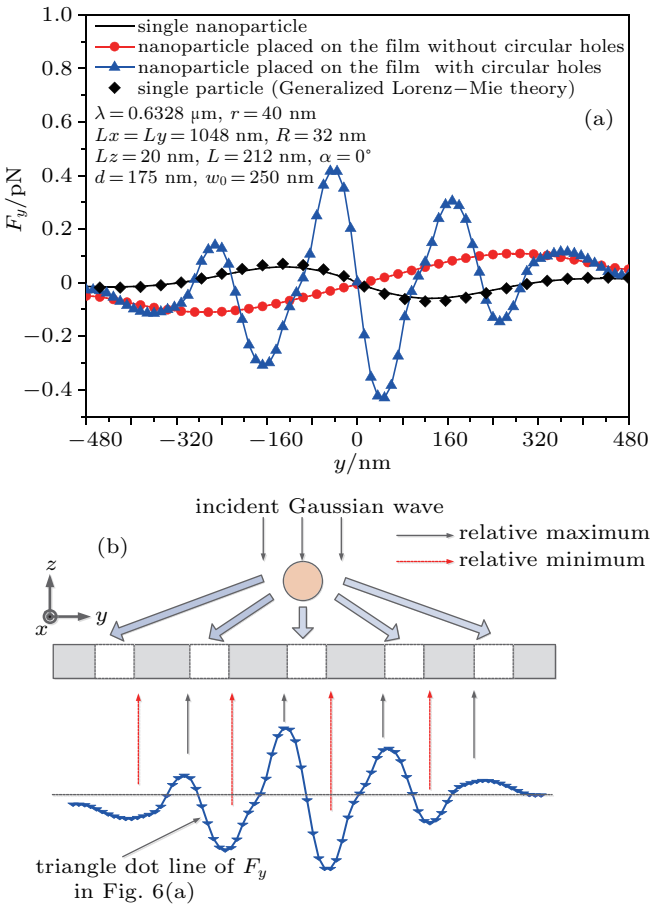


Fig. 6. Single nanoparticle and single nanoparticle placed on film with and without circular holes: (a) Lateral optical trapping force F_y, and (b) characteristic diagram of optical trapping force exerted on nanoparticle placed on the film with periodic circular holes.

As shown in Fig. 6(b), the SPPs are more effective to manipulate the nanoparticle, which is based on delicate equilibrium between the optical trapping forces resulting both from the incident beam and from the light re-scattered by gold film. The stable equilibriums of nanoparticle occur at the centers of the circular holes, and the scattering field of periodic circular holes is necessary to provide sufficient trapping force overcoming the forces induced by incident Gaussian beam to stabilize the stable equilibrium. The first stable equilibrium position at $y = 0$ is the most stable because it has the largest negative slope under the same influence of finite illumination area of incident Gaussian beam. These results indicate that optical trapping force exerted on nanoparticle placed on the gold film with periodic circular holes can be explained as a virtual spring[49] which has a restoring force to perform positive and negative forces as nanoparticle moves closer to or away from the centers of circular holes in the y direction. In contrast, according to Fig. 6(b), the other null force positions with a positive slope are the unstable equilibrium positions because they are equivalent to a spring with negative spring constant. The unstable equilibrium of nanoparticle occurs in the center

between two contiguous circular holes, the nanoparticle will be manipulated to the next stable equilibrium which occurs in the center of the circular hole if any disturbance occurs. Besides, the amplitude of the stable oscillation (solid line with triangles) in Fig. 6(a) is higher, which means that the gold film with periodic circular holes generates a strong scattering field. This gives rise to stronger optical interaction between nanoparticle and the film, indicating that the properties of the optical trapping force are completely controlled by the structure of gold film. The effects of various parameters on optical trapping force will be further investigated in the following.

3.3. Effects of structural parameters of gold film on optical trapping properties

To find the effects of the structural parameters of gold film on the properties of optical trapping force exerted on a nanoparticle placed on the gold film with periodic circular holes, we must consider two key parameters that affect the SPPs: the radius R and number of circular holes. The optical trapping properties of a nanoparticle placed on the gold film versus various radii of circular holes are given in Fig. 7(a). The other parameters in Fig. 7(a) are the same as those used in Fig. 6. As shown in Fig. 7(a), the position of the relative maximum and relative minimum values of optical trapping force will change with the increase of the radius of circular hole. It is clear from Fig. 5 that the SPPs will be excited around the sides of circular holes along the y axis, which means that the radius of circular hole will determine where the position of the maximum or minimum optical trapping force is. In addition, the optical trapping force becomes larger with the increase of the radius of circular hole until the radius is 60 nm. It is because the oscillations of the scattering fields on the gold film around the circular holes, which result from the interference between the fields scattered by the each circular hole, go up as the radius of circular hole increases, which gives stronger optical interaction, resulting in greater optical trapping force of nanoparticle. To illustrate the reason better, the magnitude plots for the magnetic field are presented in Fig. 7(b). The observed cross section is the same as that shown in Fig. 7(a), and the sampling point of electromagnetic field is on the gold film. In Fig. 7(b), the numerical result of magnetic field component H_z is normalized. It is clear that the electromagnetic field around the circular hole will change with the increase of the radius of circular hole. The electromagnetic field is the key factor to determine the optical trapping force, which implies that the radius of circular hole plays a crucial role in manipulating the nanoparticle placed on the film. Besides, we also notice that the variable radius of circular hole will not change the position of stable equilibrium nor unstable equilibrium of nanoparticle, which is attributed to the unchanged central position of circular hole on the gold film.

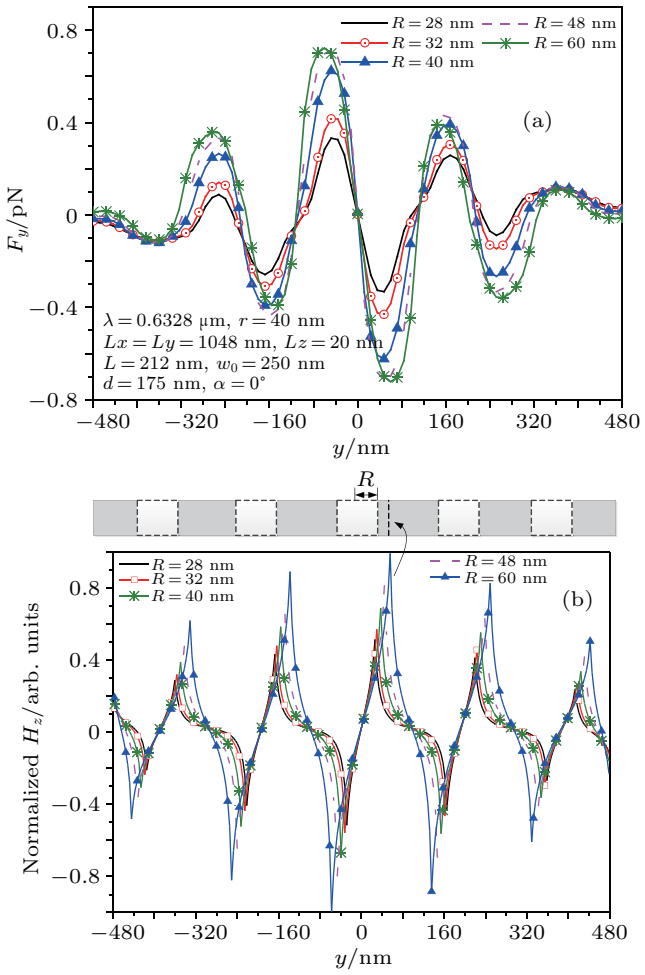


Fig. 7. Effects of different radii of circular holes: (a) optical trapping force, and (b) magnetic field component H_z.

The optical trapping properties of a nanoparticle placed on the gold film versus various numbers of circular holes are given in Fig. 8. It can be concluded that there are 3×3, 5×5, and 7×7 periodic circular holes on the gold film with fixed size. As shown in Fig. 8, the stable equilibrium position will change with the increase of the number of circular holes, which implies that the number of stable equilibrium positions is proportional to that of circular holes. The maximum and minimum value of optical trapping force will increase with the number of circular holes increasing. All of the above results show that the optical trapping force is controlled by the structure of the gold film, especially the radius and number of circular holes will affect the position and the magnitude of relative maximum value and relative minimum value of optical trapping force.

Next, numerical effects of various parameters with respect to radii of nanoparticle and beam waist, distance between incident Gaussian beam and gold film, material of nanoparticle and polarization angle of incident wave are numerically analyzed in detail. In Fig. 9(a), plotted are the results for a nanoparticle with different radii in the vicinity of the gold film

with periodic circular holes. The other parameters in Fig. 9(a) are the same as those used in Fig. 6(a). The result shows that the optical trapping force becomes larger with the increase of the radius of nanoparticle. Only a negative (positive) optical trapping force is exerted on the nanoparticle in the positive (negative) y direction when the radius of nanoparticle is larger than the diameter ($2R$) of the circular hole. In this case, the position of stable equilibrium will only occur in the center of the gold film, which implies that the nanoparticle will not be trapped by the other circular holes. This happens because the intensity of SPPs that is excited at the other position of circular holes is not enough to trap the nanoparticle. With the further increase of radius of nanoparticle, the optical trapping properties will gradually tend to be that for the case of single nanoparticle, which is similar to the black line in Fig. 6(a). Hence, to effectively manipulate the nanoparticle in the vicinity of the gold film with periodic circular holes, the radius of nanoparticle cannot be larger than the diameter of circular hole.

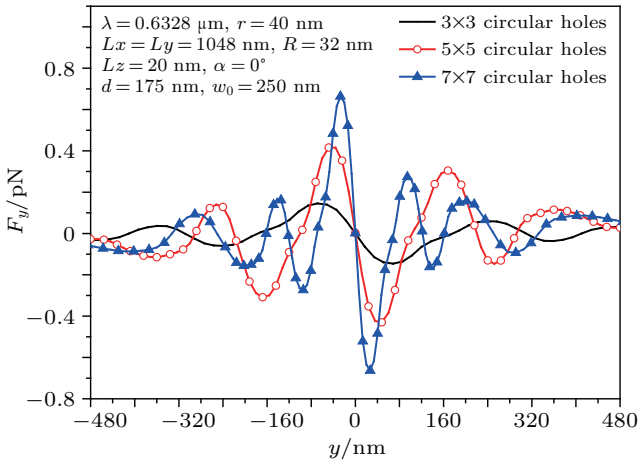


Fig. 8. Effects of different numbers of circular holes on optical trapping force.

Figure 9(b) plots the results for the incident Gaussian beam with different beam waist radii, with the other parameters remaining unchanged. According to the results in Fig. 9(b), when beam waist radius increases, the optical trapping force becomes larger, and constant amplitude of the oscillation seems to emerge if the beam waist radius increases beyond a certain threshold. As shown in Fig. 9(b), the maximum value and minimum value of the optical trapping force which is around the central circular hole tend to be constant when the beam waist radius is more than 350 nm, the secondary maximum value and secondary minimum value of optical trapping force also tend to be constant when the beam waist radius is more than 450 nm. These results indicate that optical trapping force will have a limit value under the condition of fixed structure parameters. With the increase of beam waist radius, the optical trapping force around each circular hole will be constant and gradually become stable due to the fixed intensity of incident electric field. In addition, the beam waist radius of incident Gaussian beam will not change the position of stable equilibrium with respect to the zero force, which implies that the beam waist radius of the incident Gaussian beam only influences the magnitude of optical trapping force. Hence, it can be concluded that the structural parameters of the gold film are more effective than those of incident wave to determine the optical trapping properties of nanoparticle.

To find the effects of distance between incident Gaussian beam and gold film, the properties of optical trapping force varying with distance d are shown in Fig. 9(c). As shown in Fig. 9(c), the usual oscillation of the force results from the interference between the field scattered by the nanoparticle and gold film as the distance d varies, while the amplitude of the oscillation is directly related to the strength of optical trapping force. It is clear that the variation of distance d can significantly affect the magnitude of optical trapping force acting on a nanoparticle, which implies that the larger d will reduce the potential of manipulation exerted on nanoparticle. It is because SPPs are surface electromagnetic excitations that are determined by the interaction between gold film and incident wave, the larger distance d can reduce this interaction. The combination of Fig. 9(b) with Fig. 9(c) provides us a significant idea that the distance d and beam waist radius have the same effect on optical trapping properties, which implies that the distance d and beam waist radius only affect the magnitude of optical trapping force. These results can help us to reliably manipulate the nanoparticle in the vicinity of the gold film with periodic circular holes.

Furthermore, nanoparticles of different materials have been used as the target to investigate the scattering contribution of nanoparticle in a composite structure. Figure 9(d) shows the results for nanoparticles of different materials placed on the gold film. The other parameters in Fig. 9(d) remain unchanged. According to the results in Fig. 9(d), it is clear that ordinary dielectric nanoparticle has few effects on its own optical trapping properties, which implies that the scattering field of ordinary dielectric nanoparticle is slight compared with SPPs excitations that propagate along the surface of the gold film. These results are consistent with the advantages that SPPs are more effective to manipulate the nanoparticle in the vicinity of gold film with periodic circular holes. Besides, the scattering contribution of the nanoparticle for gold material is larger than that for the case of ordinary dielectric material, and the overall effect of gold nanoparticle is to increase the magnitude of the optical trapping force. This is due to the existence of localized surface plasmon which makes its own electromagnetic field much larger on the surface of the gold nanoparticle, leading to the scattering contribution on the optical trapping force.

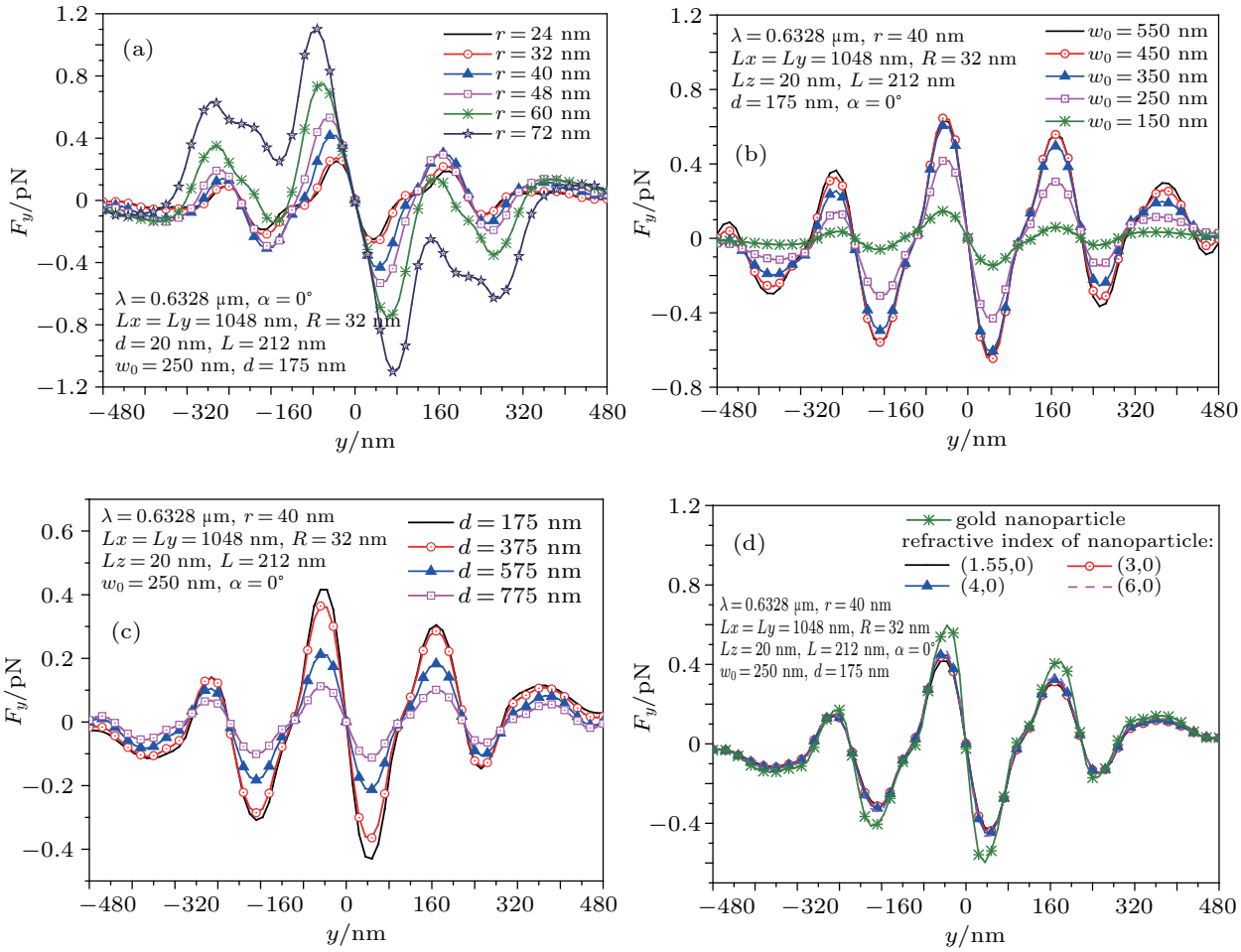


Fig. 9. Effects of structural parameters of gold film on optical trapping force for the cases: (a) different radii of nanoparticle placed on the gold film, (b) different beam waist radii, (c) different distances between center of Gaussian beam and gold film, and (d) different materials of nanoparticle placed on gold film.

In this paper, the optical trapping force can be explained as a virtual spring that has a restoring force to perform positive and negative force as nanoparticle moves closer to or away from the center of circular hole in the y direction under the illumination of Gaussian beam of linear polarization. So, it is crucial to investigate the effect of polarization angle α on optical trapping force. Figure 10 shows the effects of different polarization angles of incident Gaussian beam on optical trapping properties, where the other parameters in Fig. 10 are the same as those used in Fig. 6(a). We study theoretically how the optical trapping force depends on the polarization angle. According to Fig. 10, the optical trapping properties will be reversed by changing the polarization angle from 0° to 90°. The exchange of the positions of stable equilibriums and unstable equilibriums will happen with the polarization angle increasing. We also note that the force in $\alpha = 90°$ polarization is larger than that in $\alpha = 0°$ polarization, which is attributed to sensitive interaction between incident wave and gold film when the incident electric field along the moving direction of nanoparticle ($\alpha = 90°$). To better illustrate the properties with different polarization angles, figure 11 shows the distribution of the magnetic field component H_z. This indicates that the direction of SPPs will change correspondingly with the change of polarization angle. So, it can be concluded that the optical trapping force can be switched between positive trapping and negative trapping by changing the polarization angle, and the positions of stable equilibriums and unstable equilibriums can also be switched by utilizing the different polarization angles.

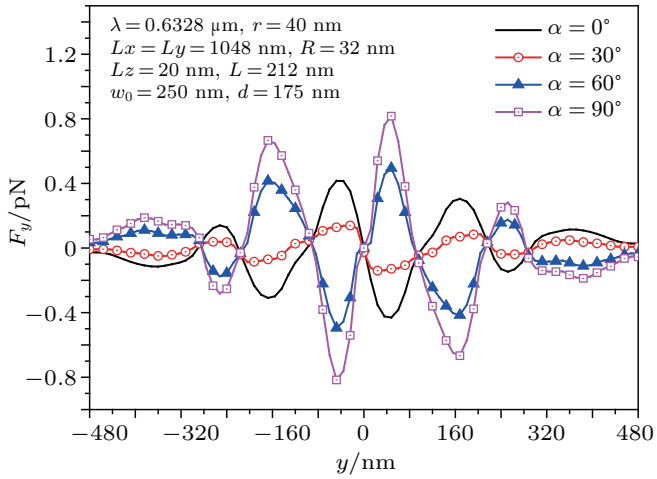


Fig. 10. Effects of different polarization angles on lateral optical trapping force.

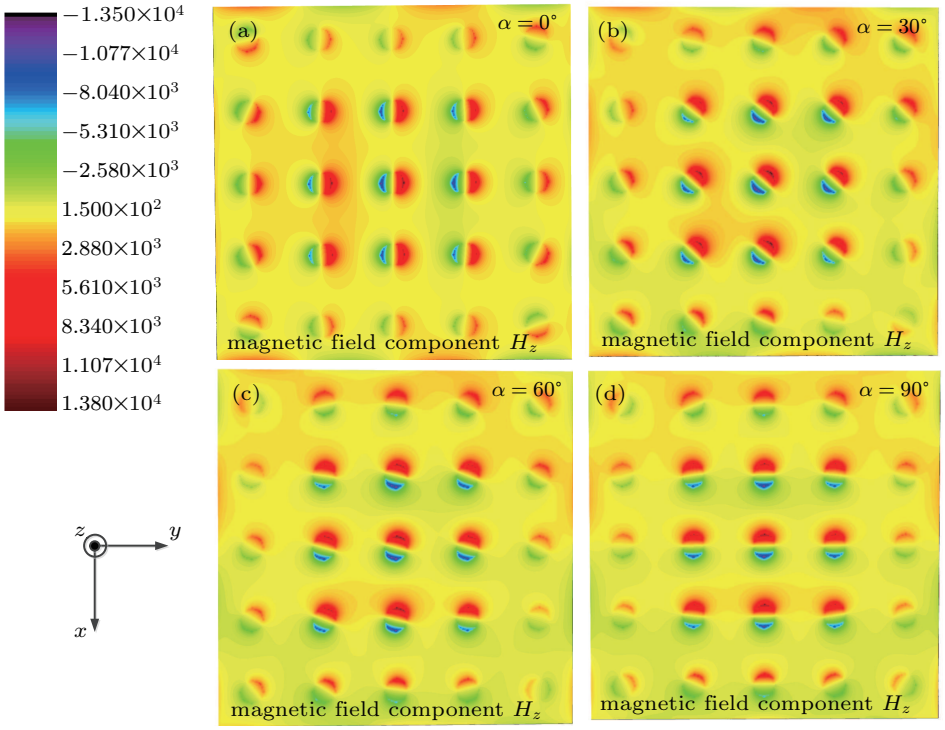


Fig. 11. Distribution of magnetic field component H_z on gold film with different polarization angles: (a) $\alpha = 0°$, (b) $\alpha = 30°$, (c) $\alpha = 60°$, and (d) $\alpha = 90°$.

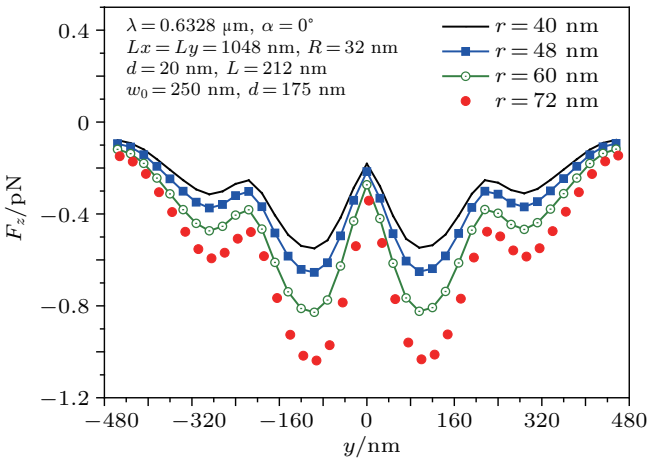


Fig. 12. Effects of nanoparticle size on longitudinal optical trapping force Fz (along the beam axis) exerted on nanoparticle placed on gold film with periodic circular holes.

Finally, the effect of the size of nanoparticle on the properties of longitudinal optical trapping force (along the beam axis) is numerically investigated to demonstrate that the properties of longitudinal optical trapping force are similar to those of lateral optical trapping force. Figure 12 shows the longitudinal optical trapping properties with different radii of nanoparticle. The parameters in Fig. 12 are the same as those used in Fig. 6(a). This result indicates that the size of nanoparticle has an influence on the magnitude of longitudinal optical trapping force. The most important in all the cases in Fig. 12 is that the longitudinal optical trapping force is always negative, no matter where the nanoparticle is. It can therefore be concluded that the nanoparticle will be manipulated to move toward the composite gold film and become bound on the surface, which implies that the properties of lateral optical trapping force F_y in the horizontal direction is more intriguing in this paper. Hence, all the results which are investigated based on lateral optical trapping force F_y in Section 3 are valid and can provide guidelines for the manipulation of arbitrary nanoparticles.

4. Conclusions

In this paper, the calculation model of the composite structure is established by using 3D dispersive FDTD method to investigate the optical trapping force properties of a nanoparticle in the vicinity of the gold film with periodic circular holes. Maxwell stress tensor is added into the calculation model to solve the problem of accurate calculations of optical trapping force. The accuracy of the calculation model in this paper is verified by comparing our numerical results with the results obtained by generalized Lorenz–Mie theory given by the literature. This calculation model is better than the other methods because of its wide range of applications. Once various conditions of FDTD method are set up correctly, this calculation model can be applied to a number of research problems. In this work, the effects of various cases on the optical trapping force are investigated in detail, which can help us open up possibilities for manipulating the nanoparticle more accurately and reliably. Our results indicate that the SPPs play a crucial role in manipulating the nanoparticle. Lateral optical

trapping force exerted on nanoparticle can be explained as a virtual spring which has a restoring force to perform positive and negative forces as nanoparticle moves closer to or away from the center of circular hole (stable equilibrium). Additionally, the effects of the structural parameters on the optical trapping properties are investigated. These results show that the radius of circular holes will determine where the position of the maximum or minimum optical trapping force is. There is only negative (positive) optical trapping force exerted on the nanoparticle in the positive (negative) y direction when the radius of nanoparticle is larger than the diameter ($2R$) of the circular holes. The beam waist radius and the distance between incident Gaussian beam and gold film only affect the magnitude of optical trapping force. For the cases of different material nanoparticle, the effect can be valid when the localized surface plasmon is excited on the surface of gold nanoparticle. Finally, the optical trapping force can be switched between positive trapping and negative trapping by changing the polarization angle, and the positions of stable equilibriums and unstable equilibriums can also be switched by utilizing the different polarization angles. The above results can provide a theoretical basis for optical system design, and they are helpful for manipulating the nanoparticle. However, further investigations are still required before reaching the final goal. In the program compilation (C++), the time taken for the numerical calculation depends on the step length of moving nanoparticle, size of composite gold film, discrete grid, *etc*. In this paper, it takes about 18 min to calculate out the optical trapping force exerted on nanoparticle at each point with WIN10 x64 system (I5-7400 CPU 8-GB RAM), which will be accelerated by parallel computing. Therefore, it will be necessary to improve the speed of the algorithm and consider more complex cases in our future work.

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