Comparative simulation of linear polarized light focusing by dielectric microcylinders with metallic coating

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Abstract. Comparative simulation of linear polarized light focusing by dielectric microcylinders with a metallic coating by finite element method implemented in COMSOL Multiphysics is presented. The analysis of simulation results shows that using two metal shells from silver and gold can decrease the spatial parameters of the focal spot.

1. Introduction

Superresolution, or overcoming the diffraction limit, which is described by the Abby theory and the Rayleigh criterion, is the theme of many fundamental and applied research in modern optics [1-5]. Tight focusing of light have the myriad of potential applications in nano-particle manipulation [6,7], super-resolution microscopy [8], biomedical devices [9], nanolithography [10], Raman spectroscopies [11], nano-structuring [12], and optical memory systems [13], etc. where a strongly localized electromagnetic wave with high intensity is desirable.

Subwavelength focal spots created by micro-optical elements are called photonic nanojets\textsuperscript{[14-16]}. Dielectric cylinders are widely used for producing nanojets. In [17] focusing of TE-polarized radiation in a region that is more than two times smaller than the diffraction limit in the two-dimensional case (the focal full width at the half maximum of the intensity was FWHM = 0.44\(\lambda\)) was shown. The focusing of light at by the dielectric (n=1.5) elliptical microcylinder with the major axis of 2.5 \(\mu\)m and a minor axis of 1.25 \(\mu\)m is simulated by using FDTD method which shows presence of photonic nanojet with smallest FWHM (230 nm) [18]. The focusing of light at by the cylinder with the major axis of 2.5 \(\mu\)m and a minor axis of 1.25 \(\mu\)m is simulated by using FDTD method. The photonic nanojet has smallest FWHM (230 nm) for the rotation angle equal to 0°. Special attention is paid to multilayer cylinders and microspheres [19-20] or to gradient elements as Luneburg lens [21-22]. The whispering gallery modes and their influence on the subwavelength light focusing were investigated in [19] by using the existing analytical solution of the diffraction problem on a cylinder. The FWHM of focal spot is equal to (0.155 \pm 0.001)\(\lambda\). Bessel-like elongated light fields was created by using a core-shell sub-wavelength spheres in [20]. The experimental implementation of a 3D Luneburg lens in the infrared band fabricated by a FsLDW technique is reported in [21]. Simulated and experimental results simultaneously exhibit interesting 3D ideal focusing performance of the 3D Luneburg lens for the infrared light at the wavelength of 6.25 \(\mu\)m.
In this paper, the focusing of laser light by dielectric cylinders with metal shells is investigated. All simulations are carried out by finite difference method (FEM) implemented in COMSOL Multiphysics software package. The wavelength of the radiation is 408 nm. As materials of core polyester and silica glass are considered. The silver and gold shells are proposed. In this paper, the focal spot characteristics, such as the maximal intensity, FWHM, depth at half maximum of intensity (DOF) are calculated for choosing optimal design.

2. Optical scheme for simulation

In this paper, the focusing by dielectric microcylinder with two metal shells is considered. However, the comparison with the ordinary dielectric cylinder is also presented. Fig. 1 shows the optical scheme of numerical simulations.

Figure 1. Simulation schem for two shell.

The core of the cylinder has the radius of \( r_D \), while the thicknesses of metal shells are \( \Delta r_{M1} \) and \( \Delta r_{M2} \) for first and second metal shells according to Fig. 1. The core radius is fixed and equal to 2.5 \( \mu m \). The total thickness of both shells is chosen equal to 10 nm according to our previous investigations [22].

At this study, several materials for the core of microcylinder are considered. The first one is silica glass which refractive index is \( n_{SiO2} = 1.41 \). Another material is polyester with \( n_P = 1.59 \). Silver and gold were chosen as materials of the shells. Dielectric permittivity of metals is described by the Drude-Lorentz model [23]:

\[
\varepsilon_m(\omega) = \varepsilon_\infty + \frac{\omega_p^2}{\omega_p^2 - \omega^2 - i \omega \delta_m} + \sum_{\nu} \frac{A_\nu \omega_\nu^2}{\omega_\nu^2 - \omega^2 - i \omega \delta_\nu} \tag{1}
\]

where \( \omega \) is a frequency; \( \omega_p \) is the plasma frequency; \( \nu \) is the collision frequency; \( A_\nu \) is the resonance strength; \( \delta_m \) is the damping factor; \( \omega_\nu \) is the resonant frequency. Tables 1 and 2 show parameters for the Lorentz's part of permittivity model of silver and gold, respectively. Drude's part of permittivity model has next values: \( \varepsilon_\infty = 1 \), \( \omega_p = 41.94605 \) Hz, \( \nu = 0.243097 \) Hz and \( \varepsilon_\infty = 1 \), \( \omega_p = 39.86873 \) Hz, \( \nu = 0.13421 \) Hz for silver and gold, respectively.

TM-polarized laser pulse with wavelength of \( \lambda_0 = 405 \) nm is considered as incident light. The following values of the refractive index \( n_{Si} = 1.46 + 1.945i \) and \( n_{Ag} = 0.05 + 2.168i \) are obtained at considered wavelength for silver and gold, respectively.

| \( m \) | \( A_\nu \) | \( \delta_\nu, \text{Hz} \) | \( \omega_\nu, \text{Hz} \) |
|---|---|---|---|
| 1 | 7.924697 | 9.840355 | 4.132646 |
| 2 | 0.501327 | 1.144581 | 22.6941 |
| 3 | 0.013329 | 0.164597 | 41.45307 |
| 4 | 0.826552 | 2.319549 | 46.001 |
| 5 | 1.113336 | 6.125 | 102.759 |
3. Results of FEM simulations for TM-polarized light

In this part, the results of FEM simulations for TM-polarized laser beam carried out by the COMSOL Multiphysics package are presented. Here and after irregular grids with variable steps are used. A small step equal to $\lambda/80$ is used in regions which are close to the interface between two media (metal/dielectric or metal/metal) while the other area is described by grids with steps of $\lambda/40$. While the simulations such focal spot parameters as a focal length $f$, the maximum intensity $I_{\text{max}}$, the full width at the half maximum of intensity $FWHM_x$, and the depth of the focus at half maximum of intensity $DOF_z$ are analyzed. Results are presented in Tables 3-4.

It can be seen from Table 4 that the gold film leads to a strong decreasing of intensity (3 times). However, this design allows to obtain the most compact focal spot. Using a silver shell also leads to a decreasing of the maximum intensity at the focus (1.35 times). Using two metal layers in a dielectric coating allows to compensate the influence of gold. In this case, the maximal intensity in the focus is smaller in two times. Significant changes in the spatial parameters of nanojets are not observed, however, the width and depth of focus are nominally reduced. In addition, in the case of using silver in the first layer and gold in the second allows to obtain a tighter spot with a larger maximum intensity in comparison with the design which uses reverse order of materials in the shells.

It can be seen from Table 4 that the gold film again leads to a strong decreasing of intensity (3 times). However, this design allows to obtain the most compact focal spot. Using a silver shell also leads to a decreasing of the maximum intensity at the focus (1.28 times) and increasing of FWHM of the focal spot. It can be noticed that the focus is shifted by 150 nm from the cylinder boundary. Using two metal layers in a dielectric coating allows to compensate the influence of gold. In this case, the maximal intensity in the focus is smaller in two times and the focus shifts by 100 nm from the cylinder boundary. Significant changes in the spatial parameters of nanojets are not observed, however, the width and depth of focus are nominally reduced. In addition, in the case of using gold in the first layer and silver in the second allows to obtain a tighter spot with a larger maximum intensity in comparison with the design which uses reverse order of materials in the shells.

### Table 2. Parameters for the Lorentz’s part of gold permittivity model [24].

| m  | $\omega_m$, Hz | $\delta_m$, Hz | $\sigma_m$, Hz |
|----|----------------|----------------|---------------|
| 1  | 11.36293       | 0.610274       | 2.101774      |
| 2  | 1.183639       | 0.873629       | 4.203549      |
| 3  | 0.65677        | 2.203065       | 15.03655      |
| 4  | 2.645486       | 6.315          | 21.79768      |
| 5  | 2.014826       | 5.60642        | 67.45936      |

### Table 3. Simulation results for microcylinder with core from polyester.

| $\Delta r_{M1}$, nm | $\Delta r_{M2}$, nm | $f$, nm | $I_{\text{max}}$, a.u. | $FWHM_x$, nm | $FWHM_z$, nm | $DOF_x$, nm | $DOF_z$, nm |
|---------------------|---------------------|--------|------------------------|--------------|--------------|--------------|--------------|
| -                   | -                   | 380    | 14.47                  | 282.8        | 0.70         | 915.3        | 2.26         |
| 5 (Au)              | 5                   | 380    | 7.07                   | 282.2        | 0.70         | 880.4        | 2.17         |
| 5 (Ag)              | 410                 | 7.12   | 280.0                  | 0.69         | 873.2        | 2.15         |
| 10 (Au)             | -                   | 390    | 4.73                   | 280.1        | 0.69         | 856.0        | 2.11         |
| 10 (Ag)             | -                   | 400    | 10.66                  | 282.3        | 0.70         | 907.7        | 2.24         |

### Table 4. Simulation results for microcylinder with core from silica glass.

| $\Delta r_{M1}$, nm | $\Delta r_{M2}$, nm | $f$, nm | $I_{\text{max}}$, a.u. | $FWHM_x$, nm | $FWHM_z$, nm | $DOF_x$, nm | $DOF_z$, nm |
|---------------------|---------------------|--------|------------------------|--------------|--------------|--------------|--------------|
| -                   | -                   | 920    | 12.71                  | 299.2        | 0.74         | 1445.1       | 3.57         |
| 5 (Au)              | 5                   | 1015   | 6.16                   | 296.4        | 0.73         | 1320.1       | 3.26         |
| 5 (Ag)              | 5                   | 1015   | 6.12                   | 296.4        | 0.73         | 1358.5       | 3.35         |
| 10 (Au)             | -                   | 978    | 3.94                   | 293.6        | 0.72         | 1314.8       | 3.25         |
| 10 (Ag)             | -                   | 1075   | 9.95                   | 302.2        | 0.75         | 1344.2       | 3.32         |
Figure 2 shows the intensity distribution in the focal plane for cases which are marked by color in Tables 3-4.

![Figure 2](image.png)

**Figure 2.** The intensity distribution along the X axis in the focal spot (a) and along the Z axis at x = 0 (b) after the TM-polarized beam propagating through a dielectric cylinder with two metal shells. Blue line depicts simulation results for optimal parameters from Table 3 for polyester microcylinder. Red line depicts simulation results for optimal parameters from Table 4 for microcylinder from silica glass.

Comparing of two designs can show that using polyester in the core of microcylinder allows to get narrowest photonic nanojets with maximal intensity. However photonic nanojets produced by cylinders from silica glass has bigger DOF_z which exceeds 1.5 times the length of nanojets formed by the polyester cylinder. The microcylinder with the core from silica glass also has bigger focal length. It can be useful in different application.

### 4. Results of FEM simulations for TE-polarized light

In this part, the results of FEM simulations for TE-polarized laser beam carried out by the COMSOL Multiphysics package are presented. The analogous investigation of focal spot parameters is provided. Similar grids are used for calculation. The results of analogous analyzes of focal spot parameters are presented in Tables 5-6.

**Table 5.** Simulation results for TE-polarized light and core from polyester.

| Δr_{M1}, nm | Δr_{M2}, nm | f, nm | I_{max}, a.u. | FWHM_x, nm | FWHM_y, λ | DOF_z, nm | DOF_z, λ |
|-------------|-------------|-------|---------------|-------------|------------|-----------|----------|
| -           | -           | 330   | 17.18         | 204.6       | 0.51       | 865.2     | 2.14     |
| 5 (Au)      | 5           | 300   | 7.06          | 208.2       | 0.51       | 847.5     | 2.09     |
| 5 (Ag)      | 5           | 310   | 6.96          | 209.0       | 0.52       | 848.9     | 2.10     |
| 10 (Au)     | -           | 315   | 4.35          | 210.4       | 0.52       | 884.7     | 2.18     |
| 10 (Ag)     | -           | 295   | 11.82         | 202.4       | 0.50       | 756.4     | 1.87     |

It can be seen from Table 5 that the tightest focal spot is formed by the microcylinder with a silver shell. The maximal intensity in the focal spot is smaller than in the case of ordinary microcylinder without shell only in 1.45 times. The tendency of metal shell influence which is described in previous cases saves: the can help decrease spatial parameters of the focal spot.

**Table 6.** Simulation results for TE-polarized light and core from silica glass.

| Δr_{M1}, nm | Δr_{M2}, nm | f, nm | I_{max}, a.u. | FWHM_x, nm | FWHM_y, λ | DOF_z, nm | DOF_z, λ |
|-------------|-------------|-------|---------------|-------------|------------|-----------|----------|
| -           | -           | 920   | 14.97         | 234.2       | 0.58       | 1227.1    | 3.03     |
| 5 (Au)      | 5           | 880   | 5.42          | 256.6       | 0.63       | 1401.3    | 3.46     |
| 5 (Ag)      | 5           | 890   | 5.53          | 262.2       | 0.65       | 1396.2    | 3.45     |
| 10 (Au)     | -           | 900   | 3.20          | 262.6       | 0.65       | 1456.4    | 3.59     |
| 10 (Ag)     | -           | 890   | 10.06         | 258.2       | 0.64       | 1332.3    | 3.29     |

It can be seen from Table 6 that the most appropriate results gives an ordinary microcylinder without any shells. However, using metal coatings leads to an increasing of nanojets DOF but at the same time, the maximal intensity is decreasing. As in a previous investigation for the TM-polarized
light gold film leads to the most strong decreasing of intensity (3 times). Table 6 shows that presence of metal shell can increase the DOF of photonic nanojet.

Figure 3 shows the intensity distribution in the focal plane for cases which are marked by color in Tables 3-4.

![Figure 3](image)

**Figure 3.** The intensity distribution along the X axis in the focal spot (a) and along the Z axis at x = 0 (b) after the TE-polarized beam propagating through a dielectric cylinder with two metal shells. Blue line depicts simulation results for optimal parameters from Table 5 for polyester microcylinder. Red line depicts simulation results for optimal parameters from Table 6 for microcylinder from silica glass.

Comparing of two designs shows that as in a previous case using polyester in the core of microcylinder is preferable. In both cases of linear polarization, these microcylinders allow to get narrowest and intensive focal spot. At the same time, TE polarization gives smaller focal spots than TM polarization. Using metal shells can help to decrease spatial parameters of the focal spot while the maximal intensity falls only in 1.5 times.

5. Conclusion

In this paper, we consider the focusing of laser light by multilayered microcylinder. All simulation is carried out by FEM which is realized in COMSOL Multiphysics software package. The radius of the cores was equal to $r = 2.5 \, \mu m$. The wavelength of the incident light was 405 nm. Different types of materials were used for core and shells of microcylinder. The simulation shows that polyester is more useful for light focusing. For TM-polarized light using of two metal shells from silver and gold can decrease spatial parameters of photonic nanojet while maximal intensity falls only in 1.5 times. In the case of TE-polarized light using of the metal coating is justified only in the case of a polyester core, while in the case of silica glass the optimal characteristics have the focal spot formed by ordinary microcylinder without shells.

6. References

[1] Kozawa Y, Matsumaga D and Sato S 2018 Optica 5 86-92
[2] Chang-kun S, Zhong-quan N, Yan-ting T, Chao L, Yong-chuang Z and Bao-hua J 2018 Optoelectronics Letters 14 0001-0005
[3] Astratov V N, Maslov A V, Allen K W, Farahi N, Li Y, Brettin A, Limberopoulos N I, Walker D E, Urbas A M, Liberman V and Rothschild M 2016 Proc. SPIE 9721 97210K
[4] Savelyev D A and Khonina S N 2015 Characteristics of sharp focusing of vortex Laguerre-Gaussian beams Computer Optics 39(5) 654-662 DOI: 10.18287/0134-2452-2015-39-5-654-662
[5] Kozlova E S and Kotlyar V V 2013 Simulation of focusing femtosecond pulse by ellipsoid, paraboloid, sphere and hemisphere Computer Optics 37(1) 31-38
[6] Taylor M A, Janousek J, Daria V, Knittel J, Hage B, Bachor H-A and Bowen W P 2013 Nature Photonics 7 229-233
[7] Porfirev A P, Kovalev A A and Kotlyar V V 2016 Optical trapping and moving of microparticles using asymmetrical Bessel-Gaussian beams Computer Optics 40(2) 152-157 DOI: 10.18287/2412-6179-2016-40-2-152-157
[8] Zhou Y, Tang Y, Deng Q, ZhaoL and Hu S 2017 Appl. Phys. Express 10 082501
[9] Astratov V N, Maslov A V, Brettin A, Blanchette K F, Nesmelov Y E, Limberopoulos N I, Walker D E and Urbas A M 2017 Proc. SPIE 10077 100770S
[10] McLeod E and Arnold C B 2008 Nature Nano 3 413-417
[11] Yi K J, Wang H, Lu Y F and Yang Z Y 2007 J. Appl. Phys. 101 063528
[12] Bhuyan M K, Velpula P K, Colombier J P, Olivier T, Faure N and Stoian R 2014 Appl. Phys. Lett. 104 021107
[13] Li X, Cao Y, Tian N, Fu L and Gu M 2015 Optica 2 567-570
[14] Mahariq I, Astratov V N and Kurt H 2016 J. Opt. Soc. Am. B. 33 535-542
[15] Geints Yu E and Zemlyanov A A 2016 J. Appl. Phys. 119 153101
[16] Kozlov D A and Kotlyar V V 2014 Resonant laser focus light by uniformity dielectric microcylinder Computer Optics 38(3) 393-396
[17] Kotlyar V V, Kovalev A A and Kozlov D A 2016 Optik 127 3803-3808
[18] Liu C-Y and Chang L-J 2014 Optik 125 4043-4046
[19] Kozlov D A, Kozlova E S and Kotlyar V V 2017 Optical Memory and Neural Networks 26 280-288
[20] Grojo D, Sandeau N, Boarino L, Constantinescu C, De Leo N, Laus M and Sparnacci K 2014 Opt. Lett. 39 3989-3992
[21] Zhao Y-Y, Zhang Y-L, Zheng M-L, Dong X-Z, Duan X-M and Zhao Z-S 2016 Laser Photonics Rev. 10 665-672
[22] Kozlova E S and Kotlyar V V 2017 Procedia Engineering 201 36-41
[23] Rakic A D, Djurisic A B, Elazar J M and Majewski M L 1998 App. Optics 37 5271-5283
[24] Vial A, Laroche T, Dridi M and Le L 2011 Appl. Phys. A. 103 849-853

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