Simovski, Constantin R.; Heydarian, Reza

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Accurate estimation of non-resonant far-field superresolution by a glass microparticle

Constantin R. Simovski, Reza Heydarian
Aalto University, Dept. Electronics and Nanoengineering, FI00076, Espoo, Finland
Tel: (+358) 50 45856, Fax: (+358) 50 45856, e-mail: konstantin.simovski@aalto.fi

ABSTRACT
In this paper, we theoretically study the spatial resolution granted by a glass microsphere to two pointwise dipoles separated by a tiny gap and located on the sphere surface. This resolution is considered via parameters of the so-called virtual sources effectively shaped by the microparticle of the radiation of the real sources. The geometrical optics qualitatively explains these virtual sources, but only full-wave simulations give a reliable information of their location and sizes. We developed a method for finding these sources from COMSOL simulations. The virtual source is defined as the waist of the wave beam obtained from the imaging beam by its exact inversion performed at a very large distance from the microparticle. We have obtained both pessimistic and optimistic estimates for the ultimate resolution. We found that the novel scenario of the microparticle imaging theoretically revealed in our previous work, promises much finer resolution than the conventional scenario.
Keywords: spatial resolution, geometrical optics, imaging wave beam, virtual source, diffraction, beam waist.

1. INTRODUCTION

When the far-field subwavelength resolution accompanied by the image magnification granted by a usual glass microsphere was experimentally revealed in [1] the unclear physics of this effect attracted a lot of attention. Scientists tried either to validate or to overturn the hypothesis of [1] that the sphere creates the virtual sources of separate object points. However, no one of early attempts was convincing. The simplistic understanding of the effect based on the geometrical optics (GO) demanded to neglect the diffraction and other wave effects, such as excitation of creeping waves, whereas the microsphere radius R is though large compared to λ is still comparable with it that makes GO not applicable, the diffraction and other wave effects not negligible. In work [2] published in 2019 very convincing numerical simulations were done for the 2D case – a glass microcylinder illuminated by line sources. These simulations revealed that the phase font of the imaging beam of the 2D point (radiation of a 2D point source transmitted through the sphere) is not homocentric at large distances and the virtual source (VS) is not formed for the imaging beam. Our idea (see e. g. in [3]) was that the VS arises in the case not covered by the simulations of [2]. Namely, GO qualitatively works if the source is polarized normally to the surface of the glass microparticle (spherical or cylindrical). Our hypothesis covered the case when GO is applicable so that to approximately predict the location of the VS. Whereas a tangentially polarized dipole creates the beam with the intensity maximum in the direction to the microscope, a normally polarized dipole creates the exact zero along imaging beam axis (the influence of the substrate to the formation of the imaging beam is negligibly small, and the problem can be treated as an axially symmetric one). The axis of the imaging beam restricts the diffraction of the imaging beam in free space. The information on the lateral location of the point source is kept in its imaging beam at whatever distances because this location is pointed out by the beam axis (by the intensity zero). This way the diffraction limit is beaten, and the VS really can be formed for such the imaging beam.

We reproduced the simulations of [2] and added the case of normally polarized dipole lines. Indeed, for the tangential polarization of the source when the glass cylinder is excited by the current line the diffraction spread of the energy in the imaging beam is not restricted and the imaging beam (which is approximately homocentric at a small distance from the cylinder) loses the properties of the cylindrical wave at the Rayleigh range D_R from the cylinder. In this case, the VS is not formed. Meanwhile, for the normally polarized source we found a wide range of refractive indices n and cylinder radiuses R for which the imaging beam at very large distances keeps nearly homocentric. In this work, we report our study of VSs for two scenarios of microparticles nanoscopy and give the estimates for the spatial resolution based on full-wave numerical simulations for the 2D case. We also explain why the image formed by the useful (radial) polarization of the object may dominate over the parasitic one (tangential polarization of the object).

2. HOW TO ESTIMATE THE SPATIAL RESOLUTION

An optimistic estimate of the resolution for an object consisting of two pointwise dipoles separated by a small gap δ takes only the distance between two VSs into account. Then the ultimate resolution corresponds to the case when the gap between two VSs is equal $\lambda/2$. It may be a reasonable approach because the imaging beams created by two different sources diverge and overlapping of two VSs may be not important for the resolution. However, this is so only if two real sources are completely non-coherent. Two coherent real sources form two coherent VSs, and their overlapping may make them not distinguishable. And real sources are always mutually coherent at least partially because they are electromagnetically coupled. Therefore, another, more pessimistic approach is needed. So that to predict the interval of δ in which the ultimate spatial resolution is located we do the following pessimistic assumption. We neglect the divergence of the imaging beams and fully base the resolution on the maximal allowed intersection of VSs. If this intersection is not harmful for the key feature of two imaging beams – their axes – the real sources are resolved. This allowed intersection is nearly equal to 30% of the lateral size of the VS. So, the optimistic estimate neglects the VS size, and the pessimistic one is based solely on it.

How to simulate the VS? Seemingly, for it we need to study the evolution of the imaging beam until such distance at which the beam can be with high accuracy considered as a spherical (in the 2D case cylindrical) wave with the angular pattern. At such distances the wave beam does not experience the diffraction spread anymore and its phase front allows us to retrieve the phase centre, that we may identify as the VS. However, it is impossible to simulate the 3D imaging beam up to Rayleigh distance. Therefore, we considered the 2D case where it is possible using the supercomputer network up to the distances (10-100)$\cdot D_R$. When we did it, we saw that for a tangentially polarized dipole the diffraction spread (diffusion of the intensity along the phase front) holds in this range of distances and does not decrease with the distance. Meanwhile, for a normally polarized dipole there is a narrow paraxial region in which the diffraction spread is negligibly small, that implies the existence of the effective phase centre of such the beam -- the concept of the VS turns out to be meaningful. However, even in this case we cannot, in general, neglect the diffraction because the paraxial region in which this effect is really negligible cannot be outlined strictly. In 2D simulations reported in [3] we estimated the location of the VS neglecting the diffraction spread of the beam at the distances of the order of (1-10)$\cdot D_R$ from the glass microcylinder. We neglected the small deviation of the phase front from the ideally cylindrical one and located the VS in this heuristic way. Our further analysis has shown that we need a better method which would allow us to correctly locate the centre of the VS and to correctly find its sizes.

This method is that of the backward propagation. If we could exactly calculate the electromagnetic field on an abstract closed surface surrounding the structure (our sphere with our point source) the inversion of the magnetic field **H** on this surface would result in the inversion of the Poynting vector. Then, applying G. Green's theorem, we could restore the bulk field distribution with all features granted by the diffraction by the sphere and would restore even this sphere. However, this task is irrelevant. The image is formed in the microscope by a small part of the imaging beam – that part which illuminates the objective lens. Therefore, to restore the VS we apply the Green theorem to the finite S covering the paraxial part of the imaging beam in which most part of its power is concentrated and neglect the tails of this beam. It is important to properly find the distance y_S at which we take this surface. In our simulations we increased y_S until the stable result for the VS is obtained i. e. the coordinate of the VS y_W does not change for larger y_S.

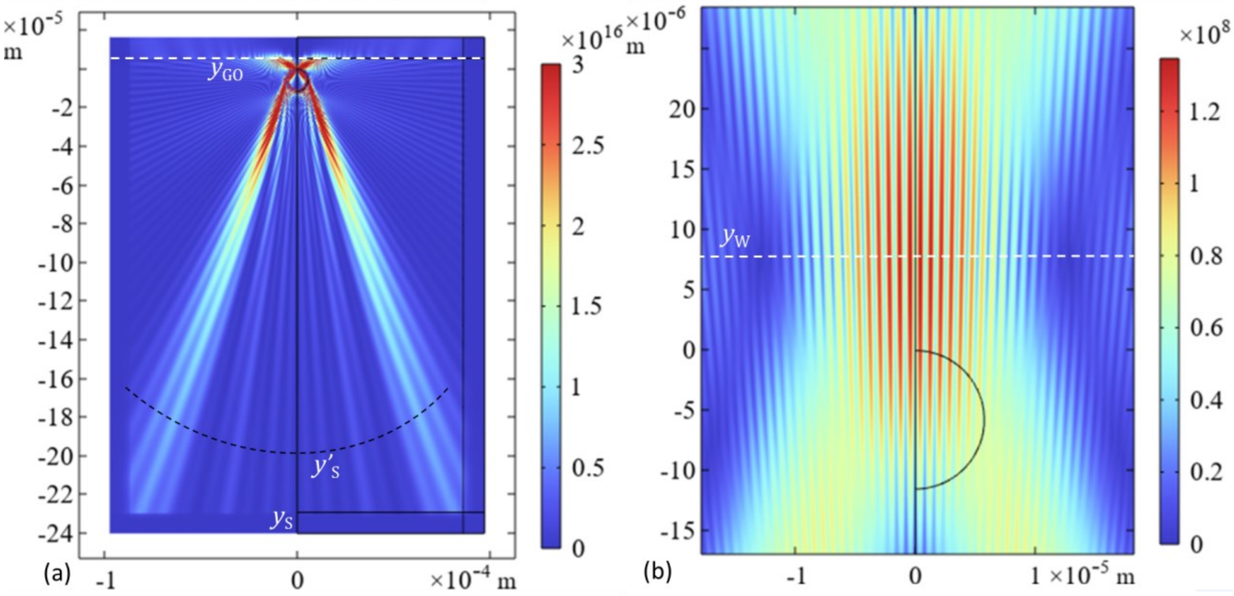

Figure 1. The case R=4.3λ, n=1.35, *when the VS is formed at the real source side: (a) – intensity colour map in area of the imaging beam, (b) – intensity colour map of the backward beam in the area of the VS. In the case when the VS is located like this we have* $y_W \approx y_{GO}$ *and the conventional scenario of nanoimaging is implemented.*

The VS is the waist of this backward beam. It is so because in this waist the beam phase front is practically flat and both **E** and **H** fields are tangential (E=E_x, H=H_z). Therefore, the inversion of **H** allows us to restore the imaging beam with the excellent accuracy but without parasitic sidelobes and backscattered waves that we see in Fig. 1(a). The case presented in Fig. 1 corresponds to following parameters of the microcylinder (recall that our simulations are 2D): n=1.35 (refractive index), R=2.37 μm (radius), and λ=0.55 μm. In this case the Rayleigh range is equal $D_R=2R^2/\lambda$=21.24 μm, that in the system whose origin x=y=0 is at the source point corresponds to the coordinate y=–26 μm, whereas minimal allowed $|y_S|$ is equal 230 μm – at order of magnitude larger than at the Rayleigh range. In this case we obtained y_W=7.7 μm (see Fig.1). Positive y_W means that the VS is located at the side of the source. We found that in all cases when the VS is formed at the source side the true location of the VS is close to that predicted by GO. If we take, for example y'_S=–200 μm and neglect the minor deviation of the real phase front at this distance from its circular approximation presented in Fig. 1(a) by a dashed line, we graphically obtain the phase centre of the imaging beam at y_{GO}=7.4 μm. In other words, in these cases the GO estimation of the ultimate δ done in [3] is valid. However, in [3] we also revealed a novel scenario of the superresolution granted by a glass microparticle. In this scenario, GO gives wrong locations of the VS.

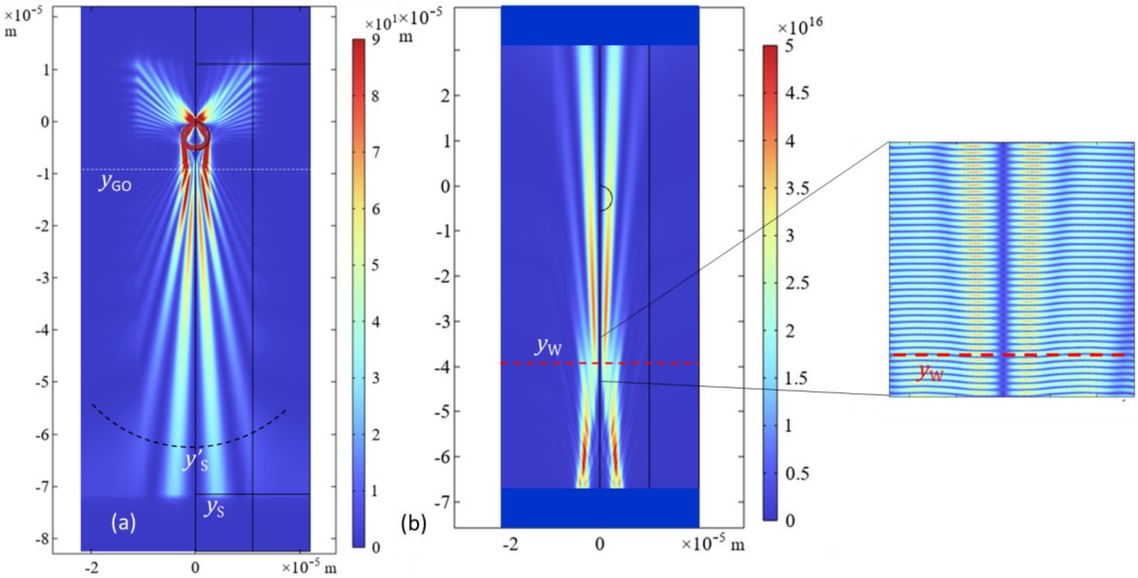

Figure 2. The case when the VS is formed at the side of the microscope (R=5λ, n=1.6): (a) – intensity colour map of the imaging beam, (b) – that of the backward beam (left panel). On the right panel an instantaneous wave picture of the backward beam is presented. At y=y_W the wave front of the backward beam is maximally flat.

This scenario corresponds to high values of n. For example, when R = (4-5)λ it holds for n>1.52. Then the imaging beam is collimated and propagates until the point y=y_{GO} without diffraction. At this point it sharply diverges and at the distances drastically exceeding D_R becomes a cylindrical wave with qualitatively similar directionality as above (two main lobes with the zero on the beam axis). Any value of $|y'_S|$ exceeding D_R delivers the VS at nearly the same point y_{GO}. However, this would be a wrong prediction for the VS location. Comparing Fig.2(a) and (b) we can see that the backward beam has the waist at y_W = –39 μm, whereas GO predicts y_{GO}= –9.5 μm. The farther is the location of the VS from the real source the larger is magnification, and, therefore, the finer is the ultimate resolution. In Table 1 we present the values of the ultimate resolution calculated with the optimistic approach (δ corresponding to the gap λ/2 between the centres of the VSs) and with the pessimistic approach (δ corresponding to the 30% intersection of the VSs) for two values of n, and two values of R selected so that to avoid the Mie resonances for both n. Indeed, these bounds of the ultimate resolution correspond to the 2D case, however, we believe that they are broad enough to be valid for the 3D case.

Table 1. Pessimistic and optimistic bounds of ultimate resolution for 4 variants of a microcylinder

Non-resonant radius	Conventional Scenario (n=1.3)		Novel Scenario (n=1.6)	
R	Pessimistic estimate	Optimistic estimate	Pessimistic estimate	Optimistic estimate
4.30λ	0.72λ	0.18λ	0.38λ	0.04λ
10.45λ	0.97λ	0.39λ	0.54λ	0.05λ

3. CROSS POLARIZATION OF THE REAL SOURCES

One point remained unclear after that study. In the initial work [1] the structure comprising the flat object consisting of several nanoobjects and the glass microsphere on the same quartz substrate was illuminated by the laser light normally incident through the substrate. The subwavelength image was seen in the microscope around the touch point (of the microsphere and the substrate). In this image area the horizontal component of the object polarization (i. e. that corresponding to the incident wave polarization) is nearly tangential with respect to the sphere. Of course, the radial (normal to the sphere) component of the horizontal object polarization is nonzero and, in accordance, to our theory must create the subwavelength image, however this image should be seemingly masked by the parasitic image of the object resulting from its tangential polarization. Indeed, due to the strong diffraction spread of the imaging beam the local light intensity in this parasitic masking image would be smaller than in the subwavelength image if the tangential and normal polarization were equivalent. However, they are not. Simple estimations show: if the polarization of the object is horizontal, the intensity resulting from the tangential component of this polarization is slightly larger than that resulting from its normal component. So, in the case of the normal incidence, the subwavelength image seemingly should be veiled by the parasitic image. However, the experiments do not confirm it. To explain this point, in [4] we assumed that the veiling effect is weak due to the strong cross-polarization of the object that results from the near-field interaction between the object and the bottom surface of the microsphere. Dipole scatterers that the imaged object consists of induce two components of the glass polarization at this surface. One component is tangential, another is normal. Tangential dipoles induced by the laser light in the object and at the sphere bottom surface are parallel to one another and, in accordance with the known model of the near-field dipole coupling, interact destructively. As a result, the tangential polarization of the object decreases. Normal dipoles are collinear and interact constructively so that the object normal polarization increases. However, this hypothesis was not confirmed by full-wave simulations in [4]. These simulations were reported in our work [5] for the 2D case. In thar paper, we explained that the process of the object cross-polarization in the crevice between the substrate and the microparticle is not simple. The coupling between the nano-scatterers forming the object and the bottom surface of the glass microparticle is, though near-field, mediated by two wave processes. One is the excitation of the guided modes in the substrate. Another one is the formation of the standing wave on the substrate interface resulting from the full reflection of the wave scattered by the nano-scatterer from the microparticle touch point. Therefore, in the object area there is a region in which the tangential polarization of the object dominates. However, in the most part of the object area, the normal polarization of the object is at least not smaller than the tangential one. So, the cross-polarization effect is very significant and explains why in the case of the normal incidence the parasitic image does not veil the useful (subwavelength) image. However, for some sets of parameters the interplay between the mentioned wave processes and the quasi-static interaction results in the suppression of the cross-polarization effect. In other words, there are sets of parameters for which the normally incident light does not allow the glass microparticle to produce the far-field subwavelength image, whereas the incidence of a TM-polarized wave under sufficiently large angles should grant the superresolution.

4. CONCLUSIONS

We numerically studied the far-field subwavelength imaging by glass microparticles with the size parameter and refractive index varying in broad ranges and found the interval of values in which the ultimate resolution should be. The evident drawback of our study is the wide interval between the pessimistic and optimistic estimates for the predicted resolution. Our pessimistic criterion neglects the angle between the optical axes of the imaging beams created by two real sources. Our optimistic criterion neglects the intersection of our virtual sources, approximating them as point-wise ones. However, these estimates allow us to conclude that our original scenario of subwavelength imaging which has not yet been checked experimentally, the scenario from our work [3], in which the VS is formed at the other side of the glass microparticle, is more promising for the label-free nanoscopy than the conventional scenario. Sure, it is difficult to properly focus the microscope if we do not know the VS location even approximately (in the 3D case it is impossible to simulate it with existing numerical solvers). However, we hope that the 2D simulations of the imaging beam may predict the location of the VS in the 3D case with the sufficient accuracy for tuning the microscope, and our scenario will be experimentally implemented.

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