Numerical Simulation of the Field Confinement in a Quasiperiodic Multilayered Microsphere as an Application of the Software Engineering

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Abstract. We numerically study the peculiarities of the frequency spectrum of nanoemitters placed in a microsphere with quasiperiodic spherical stack. The spectral evolution of transmittance at the change of thickness of two-layer blocks, constructed following the Fibonacci sequence, is investigated. We found essentially nonlinear behavior of such a system: when the number of layers (Fibonacci order) increases the structure of transmittance spectrum acquires a fractal form. Our calculations show the radiation confinement and gigantic field enhancement, when the ratio of layers widths in the stack (control parameter) is close to the golden mean value. The object-oriented structure of the program (MS VS C# 2008) is discussed as an approach of the software engineering.

Key words: nanosystem, microsphere, quasiperiodic stack, numerical calculations, control of radiation.

1 Introduction

The use of microcavities and microspheres in advanced optoelectronics have provided a new view of various effects and interactions in highly integrated, functional photonic devices. A main fundamental question in this area is how to drastically increase the spectral optical field strength, using artificially produced alternating layers on a surface of microsphere. Nowadays the basic regime of the operation for bare (uncoated) dielectric microspheres is the whispering gallery mode (WGM) [1]. But since fabricating the coated dielectric spheres of the submicron sizes [2], the problem arises to study the optical oscillations in microspheres beyond the WGM regime for harmonics with small spherical numbers. These possibilities allow to expand essentially the operational properties of microspheres with attractive artificial light sources for advanced optical technologies. The important optical property of a periodic alternating spherical stack is a possibility to confine the optical radiation (see ([3]) and references therein).

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However, is periodicity necessary for such resonant optical effects?. In order to answer this question, we have studied the optical radiation of a nanosource (nanometer-sized light source), placed into a microsphere coated by a quasiperiodic multilayered structure (stack) constructed following the Fibonacci sequence. Such structures are called quasiperiodic and, lying outside the constraints of periodicity. One of the main properties of such a stack is re-reflections of the electromagnetic waves from the interfaces of the layers that result in the collective wave contributions. The collective optical effects in a quasiperiodic spherical stack are appreciated only if number of layers in the stack is large enough. In this case various approximations based on the decomposition of field states in the partial spherical modes have insufficient accuracy, so the deeper insight requires more advanced approaches. Our approach is based on the dyadic Green's function technique [5] that provides an advanced approximation for a multilayered microsphere with nanoemitters [6]. We have applied this approach to a quasiperiodic spherical stack and found the substantially enhanced optical resonances (Green function strength), when the ratio of layers width in two-layer blocks in stack (quasiperiodicity parameter) is close to the golden mean value. As far as the author is aware, the optical fields of nanoemitters placed in a microsphere with quasiperiodic spherical stack still have poorly been considered, though it is a logical extension of previous works in this area. This Report is organized as follows. In Section 2 we formulate our approach and basic equations for optical fields in a dielectric multilayered microsphere. We outline the numerical scheme of applying the dyadic Green function (DGF) technique to evaluate the spectrum of a nanoemitter placed in such a quasiperiodic system. In Section 3 outlying the structure of our object-oriented program code and the details of our program realization is discussed. In Section 4 we present our numerical results on structure of the cavity field states and resonances. In Section 5 the fractal structures of the resonances in a microsphere with quasiperiodic spherical stack dependently of the quasiperiodicity parameter is discussed. We found the enhanced field peaks if such a parameter is close to the golden mean value. In the last Section, we summarize our results.

2 BASIC EQUATIONS

A one dimensional quasiperiodic (QP) spherical stack, where a Fibonacci sequence is considered, can be constructed following a simple procedure (see e.g. [4]). Let us consider two neighbors 2 -layers segments, long and short, denoted, respectively, by **L** and **S** . If we place them one by one onto surface of a microsphere, we obtain a sequence:**LS**. In order to obtain a QP sequence, these elements are transformed according to Fibonacci rules as follows: **L** is replaced by **LS**, **S** is replaced by **L**. As a result, we obtain a new sequence: **LSL**. Iteratively applying this rule, we obtain, in the next iteration, a sequence with a five-element stack **LSLLS**, and so on. One can control the properties of such a QP stack by the use of some control parameter γ. For the stack with N-elements, where $N \gg 1$, the ratio of numbers of long to short elements is the golden mean

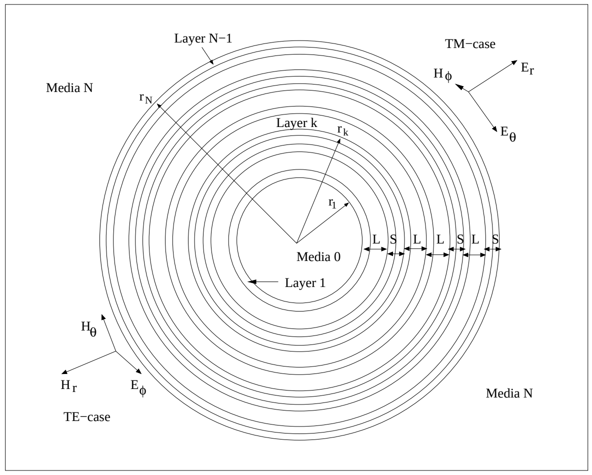

Fig. 1. Geometry of system.

value, $\Gamma_0 = 1.618$. Generally in spherical geometry the wave field depends on position of a source and it is formed on a distance scale of the order magnitude of the radius of microsphere or thickness of nanolayers of a stack. For analysis of such a spectrum it is necessary to use more advanced approach: the Green function method. The base of the latter is representation of optical field, radiated by a nanosource in a coated microsphere, as a weighed superposition (sum) of forward and backward waves (reflected from the layers interfaces). We consider a situation when radiating point source (nanoemitter) is placed into microsphere coated by a quasiperiodic stack. In this case the frequency spectrum is not described longer by a spectrum of bare microsphere slightly perturbed by the external stack. If the number of layers is large enough we have to study the photons field taking into account the spectral contributions both bottom microsphere and a quasiperiodic stack. In order to calculate the properties of such a field, we apply the Green function technique. In this case a nanosource corresponds to a nanorod or quantum dot that recently were employed in experiments with microspheres, see [10], [7] and references therein. The spatial scale of the nanoemitter objects $(\approx 1100)nm$ is in at least of one order of magnitude smaller than the spatial scale of microspheres $(10^3 - 10^4)nm$. Therefore in the coated microsphere we can represent the nanoemitter structure as a point source placed at $r\prime$ and having a dipole moment d_0. It is well known that the solution of the wave equation for the radiated electromagnetic field $E(r)$ due to a general source $J(r)$, [8], [9]

$$E(r) = i\omega\mu_0 \int_V d\mathbf{r}^{'}\mathbf{G}(\mathbf{r},\mathbf{r}^{'},\omega)\mathbf{J}(\mathbf{r}^{'}). \tag{1}$$

where $\mathbf{G}(\mathbf{r},\mathbf{r}^{'},\omega)$ is the dyadic Green function (DGF), which contains all the physical information necessary for describing the multilayered structure. Following the approach [5], we write down DGF of such a system as follows:

$$\mathbf{G}(\mathbf{r},\mathbf{r}^{'},\omega) = \mathbf{G}^{V}(\mathbf{r},\mathbf{r}^{'},\omega)\delta_{fs} + \mathbf{G}^{(fs)}(\mathbf{r},\mathbf{r}^{'},\omega) \tag{2}$$

where $\mathbf{G}^{V}(\mathbf{r},\mathbf{r}^{'},\omega)$ represents the contribution of the direct waves from the radiation sources in the unbounded medium, and $\mathbf{G}^{(fs)}(\mathbf{r},\mathbf{r}^{'},\omega)$ describes the contribution of the multiple reflection and transmission waves due to the layer interfaces. The dyadic Green's tensor $\mathbf{G}^{V}(\mathbf{r},\mathbf{r}^{'},\omega)$ in Eq.(2) is given by

$$\mathbf{G}^{fe}(\mathbf{r},\mathbf{r}^{'},\omega) = \frac{ik_s}{4\pi}\sum_{p=e,0}\sum_{m=1}^{\infty}\sum_{l=0}^{m}\frac{2m+1}{m(m+1)}x\frac{(m-1)!}{(m+1)!}(2-\delta_{01})\mathbf{G}_{pml}^{(f,e)}(\mathbf{r},\mathbf{r}^{'},\omega), \tag{3}$$

where $\mathbf{G}_{pml}^{(f,e)}(\mathbf{r},\mathbf{r}^{'},\omega)$ is the particular Green tensor, m is the spherical, l is the azimuth quantum numbers, and $k_i = \omega n_i/c$ $n_i = (\varepsilon_i(\omega))^{1/2}$ is the refraction index.

3 PROGRAM REALIZATION

Calculation of a frequency spectrum of nanoemitter radiation in a layered microsphere is a rather difficult problem in the use of computer resources, and also on the complexity of the program code organization. Our realization includes two main blocks. The first one contains the code with a description of the structure of a layered microsphere, while the second block is responsible for the dynamic calculation of a frequency spectrum and the radial distribution of an electromagnetic field in the microsphere. Other blocks of the program realize the graphic support, the data exchange, and also the mathematical library of the special functions used for evaluation of the Green function.

The organization of the program with such complexity certainly requires the object-oriented approach that provides the modularity and structure of an object-oriented computer program. It is based on several techniques, including inheritance, modularity, polymorphism, and encapsulation. In our structure (see Figure 2), the self-contained class **AbsStruct** defines the abstract characteristics of a microsphere, including its characteristics (fields or properties) and the microsphere's behaviors (methods). The base of the class hierarchy of a microsphere contains two basic classes **BaseLayer** and **BaseStack** (with general parent class **AbsStruct**); in those, the structure (materials and the sizes) of a layered microsphere is memorized. The structure of the field is described by the base class **BaseGreenTensor** that mainly contains the description of the distribution of the optical field, in terms of equation (2), and scattering matrices (arrays), used to solve equation (1).

Since a number of analytical approaches for low-layered microspheres (with 1 or 2 layers) was developed, we can compare analytical and numerical solutions

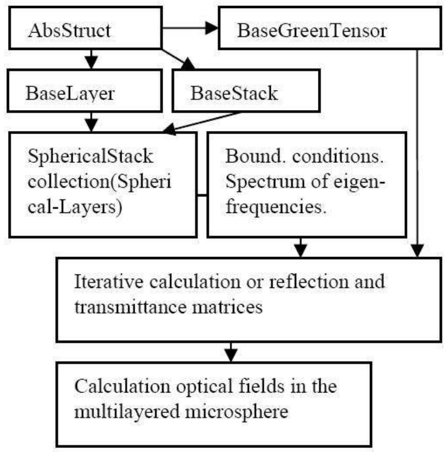

Fig. 2. The hierarchy of main classes in the program code.

to evaluate the accuracy of our calculations. To do that, we used a general conception of polymorphism that allowed us to treat derived class members (e.g. 2-layered microspheres) just like their parent class's members. More precisely, in this case the polymorphism provided us the ability to use objects belonging to different types of coated microspheres (1 or 2-layers system) to respond to method calls of methods according to an appropriate type-specific behavior.

At top of the class hierarchy, there is a class-successor *(microsphere+field)* that contains among other data two methods of the class: 1) collections of the layers that are defined by physical definition of the microsphere parameters, and 2) findings of matrixes of dispersion, calculated in agreement with the boundary conditions imposed on the field in a microsphere.

Our program has a graphic user interface (GUI) to input all parameters of a microsphere, nanoemitters and parameters of the optical fields, see Figure 3. As a result, the program calculates various dependencies, e.g., the frequency spectrum of coefficient reflection and transmittance of a stack, the spatial distribution of the optical field, real and imaginary parts of the Green function of the system, etc. The algorithm is completely realized in $C\sharp$ program language. The visualization of the frequencies dependencies is prepared by means of the package **TeeChart** ($SteemaSoftware^{(R)}$).

4 NUMERICAL RESULTS

The following parameters have been used in our calculations: the geometry of the system is $AL(B,C)...S(B,C)...D$, where letters A, B, C, and D (indicate the materials in the spherical stack), respectively. The distinct two-layered blocks $(L(B,C)$ and $(S(B,C)$ are stacked according to the Fibonacci generation rule with control parameter γ being the ratio of layers.

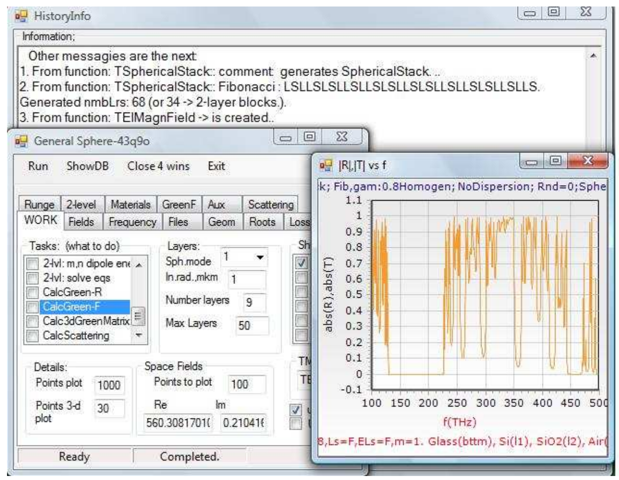

Fig. 3. Graphical user interface and example calculation of the reflection and transmittance coefficients.

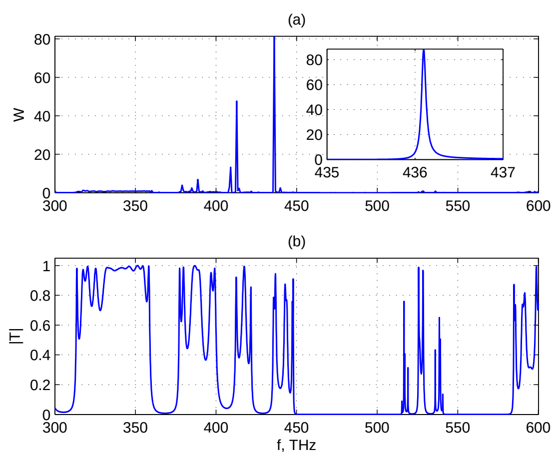

Fig. 4. (a) Imaginary parts of tangential component of the Green´s function $W = G_{\varphi\varphi}(r, r)$ for $r = 900$nm; (b) Frequency spectrum of transmittance coefficient $\mathbf{T}$ for spherical quantum number $m = 9$. Microsphere is coated by quasiperiodic stack with N=68 (34 of 2-layers blocks, order Fibonacci F_9) for $\gamma = 0.618$. See details in text.

For $\mathbf{L}$ and $\mathbf{S}$ blocks we use the notation $\mathbf{L} = (\mathbf{B}, \mathbf{C}, \mathbf{1})$ and $(\mathbf{L} = (\mathbf{B}, \mathbf{C}, \gamma)$, where γ is the ratio of both thicknesses. In order to study the behavior of the field in the microsphere, we have calculated the frequency spectrum of the transmittance coefficient $\mathbf{T}$ and the corresponding spectrum of imaginary parts of the Green's function $W \equiv Im(G_{\varphi\varphi}(\mathbf{r}, \mathbf{r}^{'}, \omega))$, where $\mathbf{r}$ is the position of a nanoemitter, and $\omega = 2\pi f$. We have calculated the evolution of a spectrum for different values γ and also for different numbers of layers in the spherical stack (Fibonacci order $\mathbf{F}_n$) for a range $[300 - 600]THz$, or $[1000 - 500]nm$. The most intensive optical peak was found for the F_9 stack, where $\gamma = 0.618 = 1/\Gamma_0(\Gamma_0 = 1.618)$ is the golden mean value). The details of the field spectra are shown in Figure 4 for 68 layers in the stack (34 of 2-layers blocks, order Fibonacci is F_9). We observe from Figure 4 that such a spectrum consists of peaks with various amplitudes; however, the most intensive peak with $W = 87$ is located at 436.1THz (details of this peak are shown in the inset). Thus, even though the periodicity of the stack is broken, well defined intensive peak of the field is clearly seen.

We have also calculated the evolution of a spectrum for different values γ close to $\gamma = 1/\Gamma_0$ for a fixed number of layers in the spherical stack (Fibonacci order F_n). The results are shown in Figure 5 for the range $[430 - 440]THz$, or $[697 - 681]nm$. One can see that in this area, the spectrum consists of rather narrow resonances, and a set of satellite peaks appears around the main peak. The intensity of this peak changes with a different γ, giving rise to another main peak, which corresponds to another quasi-periodic stack.

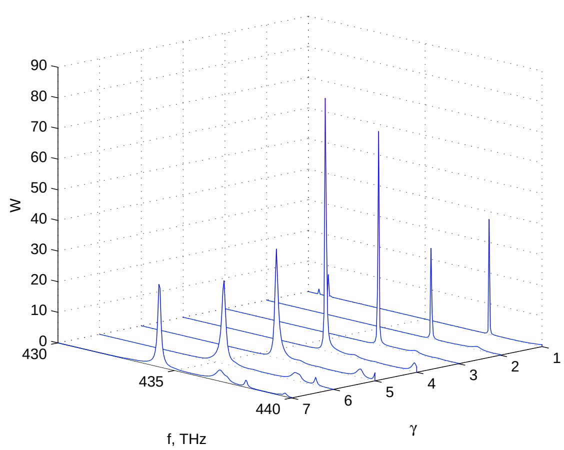

Fig. 5. Spectrum of imaginary part of the Green´s function $W = G_{\varphi\varphi}(r, r)$ for $r = 900$ nm and 68 layers in stack (34 of 2-layer blocks F_9) for different values of parameter quasiperiodisity γ close to the golden mean value: 1) 0.55, 2) 0.58, 3) 0.6, 4) 0.618, 5) 0.63, 6) 0.65, 7) 0.68.

When γ approaches to $1/\Gamma_0 = 0.618$, the field peaks become sharper, as shown in Figure 5. We observe that the amplitude of resonances is maximal for case $\gamma = 0.618$.

In previous figures, the frequency spectrum of the field ($\sim Im(G_{\varphi\varphi}(\mathbf{r}, \mathbf{r}^{'}, f))$ for the quasiperiodic stack was shown. The fractal complicity of the transmittance spectrum is defined by the intrinsic properties of the quasiperiodic spherical stack independently of the nanoemitter location. However, in experiments, it is important to identify the spatial distribution of the field radiated by nanosources located in such a quasiperiodic microsphere. Therefore, it is of interest to consider the spatial field distribution in a cross-section containing both center of the coated microsphere and nanoemitter for some resonant frequency. Such a distribution is shown in Figure 6 for the most intensive resonance at $f_0 = 436.098THz$ (see Figure 5), when the quasiperiodicity parameter $\gamma = 0.618$. We observe from Figure 6 that $Im(G_{\varphi\varphi}(r, a, \varphi)$ has a very sharp peak in the place of the nanosource location. Such a spatial field structure may be treated as a confinement of the electromagnetic energy $Im(G_{\varphi\varphi}(r, r)$ [11] inside the coated microsphere. The leakage of photons through such a structure into the outer space obviously is small.

We observe from Figure 6 that the field structure inside of the quasiperiodic stack is anisotropic and quite intricate, but the field distribution beyond the coated microsphere has a periodic character.

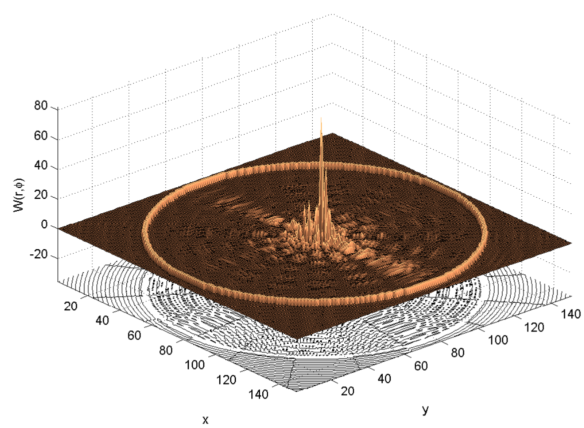

Fig. 6. Spatial structure $W(r, \varphi) = Im(G_{\varphi\varphi}(\mathbf{r}, \mathbf{r}^{'}, \omega))$ in a cross-section $0 < r < 21\mu m$ and $0 < \varphi < 2\pi$ of the microsphere with quasiperiodic stack for eigenfrequency $f =$ 436.09THz. A nanoemitter is placed at point $a = 900$nm. Other parameters are as in Figure 4. One can see the confinement of field in the stack. Outer cycle indicates the external boundary $R_{exp} = 13.8\mu$m of the quasiperiodic spherical stack.

5 FRACTAL STRUCTURE

As mentioned above, with a further increase of the Fibonacci order F_j, the structure of $|T|$ becomes more indented, see Figure 4. One can see from Figure 4(a) that in a vicinity $f = 425THz$, the splitting occurs, and here a new extreme of $|T|$ has arisen. A new maxima (and minima) reshape the initially smooth form of the transmittancy spectrum to a well expressed fractal structure. In order to calculate the fractal dimension numerically, it is normally assumed that the fractal is lying on an evenly-spaced grid; then count how many boxes are required to cover it. Such a dimension is calculated by seeing how this number changes as we make the grid finer. If $N(\varepsilon)$ is the number of boxes of side length ε required to cover the fractal, then the fractal (box-counting) dimension D_H is defined as: $D_H = lim[lnN(\varepsilon)/ln(1/\varepsilon)]$ at $\varepsilon \to 0$. Let us note that the numerical estimation D_H for a finite set is a rather difficult problem and requires a great amount of data. In our approach, we have formed the fractal by sequential elimination of quasiband gaps with values less then ε. Such an approach is similar to the Cantor set generation, where the set is created by repeatedly deleting the middle third of a set of line segments.

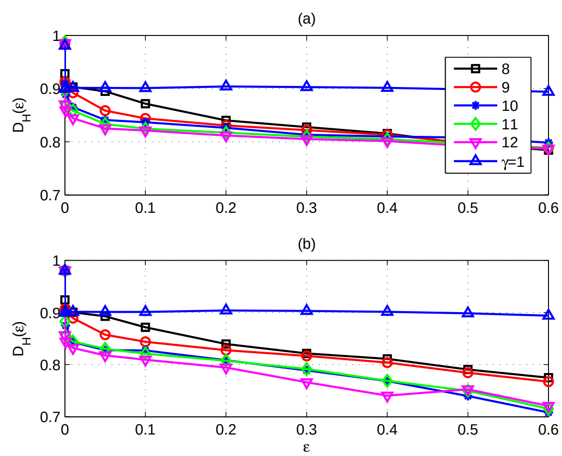

Fig. 7. Fractal (capacity) dimension $D_H(\varepsilon)$ for Fibonacci stack F_j with $j = 812$ and $\gamma = 0.5$. The last curve shows the periodic stack case with F_{12} and $\gamma = 1$. (a) lossless stack; (b) dissipative stack.

It is of interest to calculate the fractal dimension D_H for other materials in a quasiperiodic spherical stack. In particular, we studied the change of D_H for a case where the difference of refraction indexes for neighboring layers in the stack is less. We have considered D_H for stack with MgO ($n = 1.72$, 1-st layer), while the material of 2-nd layer $SiO2$ was the same as before. In this case, the difference of the refraction indexes $\Delta = 0.26$ is less with respect to the previous case. Our calculations show that the transmittance frequency spectrum for such a configuration is less indented than the previous case. Calculated fractal dimension for such a stack is $D_H = 0.965$; which is close to 1; thus the fractal properties for a stack with small Δn is less pronounced.

It is worth noting that the details of the optical field radiated by a nanoemitter incorporated into a microsphere depend on the position of such a nanoemitter. In general, such a field can be studied with the use of the above developed Green function technique. However, the latter is not necessary in a case where only the transmittance properties of a quasiperiodic spherical stack are of interest.

6 CONCLUSION

We have studied the frequency spectrum of nanoemitters placed in a microsphere with a quasiperiodic subwavelength spherical stack. We found that the transmittance spectrum of such a stack consists of quasiband gaps and narrow resonances induced by re-reflection of optical waves. We show that the width of resonant peaks in the frequency spectrum becomes *extremely narrow* for a quasiperiodic spherical stack of a high Fibonacci order. In principle, that allows creating a narrow-band filter with a transmission state within the forbidden band gap of nanoemitters, incorporated in such a coated microsphere. We have found confinement and gigantic enhancement of the optical field in a quasiperiodic structure when the ratio of layers width in two-layer blocks of the stack is close to the golden mean value. This allows us to confine resonantly the field energy in the quasiperiodic stack in a very narrow frequency range in order to create very selective stop-band filters. Incorporating nanoemitters into such structured microspheres can open new opportunities for the active control of light nanosources.

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