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Investigation of Photon Radiation in a Microsphere with Left-Handed Layers

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Abstract. The electromagnetic radiation of nanoemitters placed into a microsphere with metamaterial (dispersive left-handed -LH) layers was studied numerically. Such an investigation cannot be done analytically; it requires intensive numerical simulations with the use of the Green tensor technique and specific algorithms for the spherical functions. All of that leads to intensive consuming of the computer resources. As a result of computer experiments it is found that in the frequency range where LH layers have a negative refraction index the field frequency spectrum consists of a series of narrow and well separated resonances. In the band of such peaks, the great part of the field energy is located in a LH layer and practically does not leave the microsphere. Such conclusions were obtained as a result not only simulations, but also of a human computer interaction. We discuss the aspects of the advanced Human Computer Interaction with GUI and Usability that were developed in our study and that has allowed us to explore deeply such a complex nanosystem.

Keywords: Numerical simulations, Spherical multilayered stack.

Resumen. Se estudió numéricamente la radiación electromagnética de nanoemisores colocados en una microesfera multicapas con metamateriales con dispersión (materiles izquierdos LH). Dicha investigación no puede hacerse analíticamente, sino que requiere intensivas simulaciones numéricas con el uso de la técnica tensor de Green y algoritmos específicos para las funciones esféricas. Todo esto lleva a un intenso consumo de recursos de computo. Como resultado de los experimentos numericos se encuentra que en el rango de frecuencia donde las capas de LH tienen un índice de refracción negativo el espectro de frecuencia del campo consiste en una serie de resonancias estrechas y bien separadas. En la banda de estos picos, gran parte de la energía del campo se encuentra en una capa de LH y prácticamente no sale de la microesfera. Estas conclusiones se obtuvieron como resultado no sólo de simulaciones, sino también de una interacción persona-ordenador. Se discuten los aspectos avanzados de la Interacción Persona-Ordenador con la interfaz gráfica y usabilidad que se han desarrollado en nuestro estudio y que nos ha permitido explorar a fondo un nanosistemas complejos.

Palabras clave: Simulaciones numéricas, múlticapas esféricas.

Introduction

The recently emerging fields of metamaterials and transformation optics promise a family of exciting applications in nanophotonics with the potential for much faster information processing. The possibility of creating optical negative-index metamaterials (NIM) using nanostructured metal-dielectric composites has triggered intense basic and applied research. In very recent experiments it has been demonstrated that the incorporation of gain material in the metamaterial makes it possible to fabricate an extremely low-loss and an active optical NIM that is not limited by the inherent loss in its metal constituent. Since in such materials the electric field, the magnetic field, and the wave vector of a plane wave form a left-handed system, they are also called left-handed materials (LHMs).

1.1 Multilayered microspheres.

One of important directions is the use of microcavities and microspheres that provides a new view of various effects and interactions in structured and layered media. Nowadays, the basic regime of the operation of open (uncoated) dielectric microspheres is the whispering gallery mode (WGM) for a microsphere with a radius of the order (10-1) µm or less. The extremely high quality factors (Q-factors) $\sim 10^8 \div 10^9$ have already been realized [1-4]. But since fabricating the coated dielectric spheres of the submicron sizes, the problem arises of studying the optical oscillations in microspheres beyond the WGM regime for harmonics with small spherical numbers. The peculiarity of such a system (nanoemitter + multilayered microsphere) consists of the following. The ratio of the typical sizes of a nanoemitter (10 nm) to the typical sizes of a microsphere (1000 nm) is small ~ 0.01.

The case of the compound structure: the dielectric sphere coated by an alternative stack, is richer. The Q-factor of such oscillations strongly depends on the properties of the stack. It has a large value in the frequency regions of high reflectivity, and beyond these regions Q remains small. The combination of such factors

causes a large variety of optical properties of microspheres with a multilayer stack. In particular, such a system can serve as a spherical symmetric photonic band gap (PGC) structure, which possesses strong selective transmittance properties, and can arrange the nanometer-sized photon emitters. These possibilities allow us to essentially expand the operational properties of microspheres with the engineering of nanometer-sized photon emitters as attractive artificial light sources for advanced optical technologies.

The analysis of the refractive index properties of optical metamaterials, as a function of real and imaginary parts of dielectric permittivity and magnetic permeability demonstrated a specific interplay between the resonant responses of constituents of metamaterials that allows efficient dispersion management. Moreover, similarly constructed spherical stack allows extremely narrow frequency resonances in a quasiperiodic structure. Nevertheless, up to now, the case of a radiated nanosource placed in a LH dispersive spherical stack containing both conventional and LH materials has not been studied.

In this paper, we study this situation of a microsphere coated by alternating layers with the dispersive LH layers included. We explored both the frequency and radial dependencies of the field radiation in such a frequency area to answer the question of whether or not the spherical stack can confine the electromagnetic fields and form the new photon states. Our approach is based on the dyadic Green's function (GF) technique that provides an advanced approximation for a multilayered microsphere [5]. Such a numerical approach has allowed us to study the multilayered microspheres with any structure of the superficial layers and to evaluate the total contribution of various field states in unified framework.

2 Basic equations. The Green function.

The spatial scale of the nanoemitter objects ($1-100$ nm). at least 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 $\mathbf{r}'$ and having a dipole moment $\mathbf{d_0}$. It is well known that the solution of the wave equation for the radiated electromagnetic field $\mathbf{E}$ due to a general source $\mathbf{J}(\mathbf{r}')$ is $\mathbf{E}(\mathbf{r}) = i\omega\mu_0\mu\int_V d\mathbf{r}'\mathbf{G}(\mathbf{r},\mathbf{r}',\omega)\cdot\mathbf{J}(\mathbf{r}')$, where $\mathbf{G}(\mathbf{r},\mathbf{r}',\omega)$ is the dyadic GF, which depends on the type of boundary conditions, imposed on $\mathbf{E}(\mathbf{r})$ and contains all the physical information necessary for describing the multilayered structure. The equation for GF is complemented by the standard boundary conditions: limitation of the fields in the center of the microsphere and continuity of the tangential components of the fields at the interfaces of layers. Substituting the nanoemitter source in the form $\mathbf{J} = i\omega\mathbf{d}$ with $\mathbf{d} = \mathbf{d}_0\delta(\mathbf{r} - \mathbf{r}')$, we are obtaining the expression $\mathbf{E}(\mathbf{r}, \mathbf{r}', \boldsymbol{\omega}) = -\mathbf{p}_0\mathbf{G}(\mathbf{r}, \mathbf{r}', \omega)$, where $\mathbf{p}_0 = (\mu\mathbf{d}_0/\varepsilon_0)(\omega^2/c^2)$. In such a situation, the nanoemitter frequency spectrum is identical to the dyadic GF spectrum. Here $\mathbf{r}$ is the point where the field is observed, while $\mathbf{r}'$ is the nanoemitter (point source) location. Let us consider the multilayered spherical structure: a concentric system of spherical layers contacting with the sphere (concentric stack) deposited onto the surface of the microsphere with nanoemitters placed in such a structure. The layers are localized at the distance R_k from the center, where $d_k = R_k - R_{k+1}$ is the width of k-th layer.

2.1 Green's function of a multilayered microsphere.

Let us first specify some details of the Green's function (tensor) technique for multilayered microspheres and introduce our notations. Following the approach [6], we write down GF of such a system as fol-lows:

$$\mathbf{G}(\mathbf{r},\mathbf{r}',\omega) = \mathbf{G}^V(\mathbf{r},\mathbf{r}',\omega)\delta_{fs} + \mathbf{G}^{(fs)}(\mathbf{r},\mathbf{r}',\omega), \tag{1}$$

where $\mathbf{G}^V(\mathbf{r},\mathbf{r}',\omega)$ represents the contribution of the direct waves from the radiation sources in the unbounded medium, whereas $\mathbf{G}^{(fs)}(\mathbf{r},\mathbf{r}',\omega)$ describes the contribution of the multiple reflection and transmission waves due to the layer interfaces. Here the prime denotes the nanoemitter coordinates (r',θ',φ'), n and m are spherical and azimuthal quantum numbers, respectively, while k_s is the wave number of the medium where the radiated nanoemitters are located.

The complete equations for Green functions (tensor) are rather bulky to write here [6]. We only note that f and s denote the layers where the field point and source point are located; δ_{fs} is the Kronecker symbol, so

$$\begin{aligned}\mathbf{G}^{(fs)}_{q,nm}(\mathbf{r},\mathbf{r}',\omega) &= \Delta_{Nf}\left(\mathbf{M}^{(1)}_{q,nm}(k_f)\mathbf{P}_M + \mathbf{N}^{(1)}_{q,nm}(k_f)\mathbf{P}_N\right) \\ &+ \Delta_{1f}\left(\mathbf{M}^{(1)}_{q,nm}(k_f)\mathbf{Q}_M + \mathbf{N}^{(1)}_{q,nm}(k_f)\mathbf{Q}_N\right),\end{aligned} \tag{2}$$

Here functions M, P, N and Q are expressed with the Bessel and Hankel functions, $\Delta_{fs} = 1 - \delta_{fs}$, $k_s = n_s(\omega)\omega/c$, $n(\omega) = \sqrt{\varepsilon_s(\omega)\mu_s(\omega)}$ is the refraction index. Frequency dependent coefficients $A_k^{fs}(\omega)$, $B_k^{fs}(\omega)$, $C_k^{fs}(\omega)$ and $D_k^{fs}(\omega)$ are defined from boundary conditions and describe the details of the wave behavior in the interface of the stack layers.

2.2 The recursive calculations of the scattering coefficients.

The use of standard boundary conditions yields the relations between $A_k^{fs}(\omega)$, $B_k^{fs}(\omega)$, $C_k^{fs}(\omega)$ and $D_k^{fs}(\omega)$ coefficients that are defined by the reflection R_{jf}^k and the transmittance T_{jf}^k coefficients (in the layer interfaces) and can be written in the following recursive matrix obtaining the following form: $\mathbf{J}_k^{f+1,s} - \mathbf{I}_k^f\cdot\mathbf{J}_k^{f,s} + \boldsymbol{\sigma}^+\delta_{,f+1,s} - \mathbf{I}_k^f\cdot\boldsymbol{\sigma}^-\delta_{fs} = 0.$ The explicit expressions for the reflection R_{jf}^k and the transmittance T_{jf}^k coefficients are written in [6]. The boundary conditions for the limitation of field in the center of the microsphere and the Sommerfeld's radiation condition at $r \to \infty$. It is worth noting that due to the spherical symmetry of the system the coefficients

$A_k^{f,s}, B_k^{f,s}, C_k^{f,s}$ and $D_k^{f,s}$ are functions of *n* but not of *m*. In the following, we refer to the material of a layer as being left-handed (or metamaterial) if the real part of its refractive index is negative.

3 Numerical results.

Analytical solutions to A, B, C y D are rather laborious, and are hardly suitable in practice for studying the frequency spectrum for the cases with more than 2 layers in the stack. However, namely in such a structure, one can expect physically interesting phenomena due to the wave re-reflections in the layers of the stack. It is worth to identify the nanosource position in a microsphere. If a nanoemitter is placed close to the center of a microsphere, the system is nearly spherically symmetric; therefore the modes with small spherical quantum numbers mainly contribute to the GF. This case is close to a rotational invariant geometry where the dipole moment orientation does not need to be specified. Therefore, we draw more attention to a case where the nanoemitter is placed rather far from the center in one of the layers of the spherical stack. In such a system, the preferred direction (center-source) arises; therefore larger numbers of spherical modes contribute to DGF. As a result the frequency spectrum of DGF becomes richer but much more complicated.

3.1 The numerical scheme of applying the dyadic Green's function.

Calculation of a frequency spectrum of nanoemitter radiation in a layered microsphere is rather difficult problem on consuming 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 description of structure of a layered microsphere, while second block is responsible for dynamic calculation of a frequency spectrum and radial distribution of an electromagnetic field in the microsphere. Other blocks of program realize the graphic support, the data exchange, and also the mathematical library of the special functions used for evaluation of the function Green.

The organization of the program with such a level of complexity certainly requires the object-oriented ap-proach that provides modularity and structure of an object-oriented computer program. It is based on several techniques, including inheritance, modularity, polymorphism, and encapsulation. In our structure 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 classes 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 distribution of the optical fields and scattering matrices (arrays).

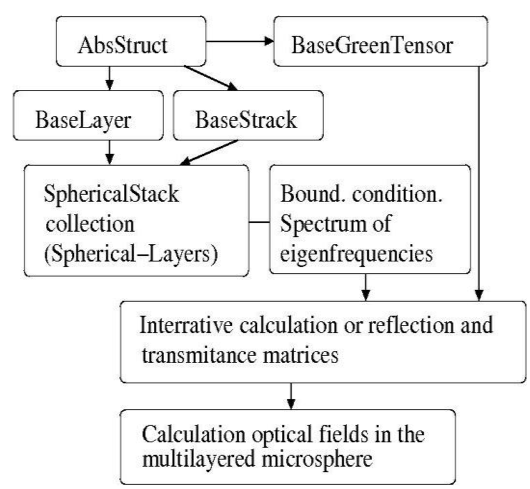

Fig. 1. The hierarchy of main classes in the program code.

Since a number of analytical approaches for low-layered microspheres (with 1 or 2 layers) were developed, we used a possibility to compare analytical and numerical solutions to evaluate the accuracy of our calculations. To do that we used a general conception of polymorphism that allowed as to treat derived class members (e.g. 2-layered microsphere) just like their parent class's members. More precisely, in this case the polymorphism provided us the ability of 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 is defined by physical definition of the microsphere parameters, and 2) findings of matrixes of dispersion, calculated in agreement with the boundary conditions imposed to the field in a microsphere.

In this Section, we briefly describe the numerical algorithm to explore the details of frequency and radial dependencies of nanoemitter radiation (the dyadic Green's function) for alternating layers deposited on the surface of a microsphere. We use the following steps: i) we solve motion equations for N -layered spherical structure; ii) we insert the calculated matrices $A_k^{f,s}, B_k^{f,s}, C_k^{f,s}$ y $D_k^{f,s}$, and finally, iii) to obtain the Green's tensor $\mathbf{G}(\mathbf{r},\mathbf{r}',\omega)$ we calculate the sums in GF expression.

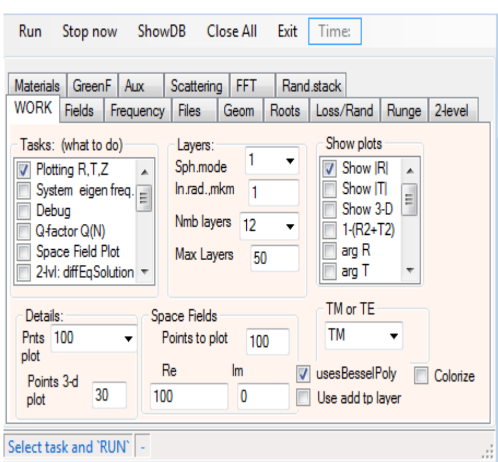

Fig. 2. Graphic user interface (GUI).

The realization of such a program requires intensive computations with the help of advanced Human Computer Interaction by means GUI. For a numerical solution, we represent GF in the form of the matrix equation $F_{ij}(a,b,c,d)=0$ with respect to the unknown boundary amplitude $a=A_k^{1,s}$, $b=B_k^{1,s}$, $c=C_k^{N,s}$ y $d=D_k^{N,s}$. Our algorithm has been constructed in such a way, that with all required coefficients the intermediate matrices $\mathbf{J}_k^{f,s}$ (which are necessary for computing the fields in the internal layers) have been calculated. Finally, this allows us to calculate the dyadic Green's tensor in any point of the spherical structure and for any number of layers in the stack, even for random structure.

3.2 The frequency spectrum of the Green's function.

The above-written approach has allowed us to explore both the frequency spectrum and the radial distribution of the Green's function in the multilayered microsphere. Some results of our calculations are shown in Fig. 3 and Fig. 4. In the user interface shown in Fig. 1, the program asks the plot of the refection and transmission coefficient or a multilayer microsphere system. The system consists of 12 layers and has a spherical number *m* = *1*. The result of this calculation is shown in Fig. 3. We can apply the program to calculate the radial distribution of the electromagnetic field. Fig. 4 shows the radial distribution $\mathbf{G}(\mathbf{r}, f)$, corresponding to the resonance frequencies of *164* THz, *165* THz and *168* THz (solid lines, with r = *1480* nm which is the position of the nanoemitter) , also shown with dotted lines the distribution of refractive indices.

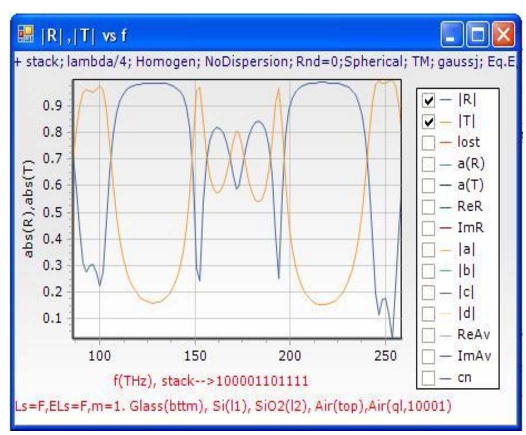

Fig. 3. Result for the reflection and transmission coefficient applied in the user interface in the Fig. 2.

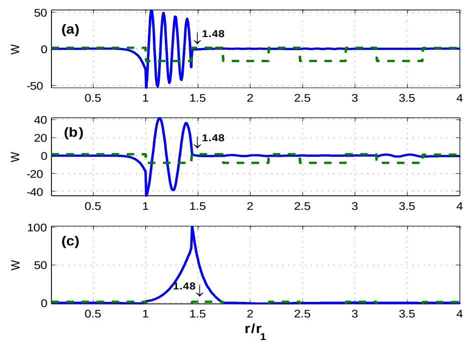

Fig. 4. Radial dependence of the imaginary part of the GF in the area of Re(n)<0. Distribution Re(n) along the stack is shown by a dashed line. We observe a confinement of the field in the first LHM layer.

4 Conclusions

We have studied the frequency spectrum and spatial dependences of the electromagnetic field (the dyadic Green's function), radiated by nanoemitters placed into the multilayered microsphere coated by the alternative quarter-wave spherical stack with LH layers included. In the area of resonances the LH layers can confine the field of nanoemitters. Such states can be very useful for quantum information technologies.

The conclusions obtained in this study are a result not only simulations, but also an advanced *Human computer interaction and usability* [7]. In our case such an interaction was realized mainly by means of advanced and friendly GUI. The code was developed in such a way that all the dependencies could be visualized in real time. This allowed working in a regime of computer experiment: a researcher could investigate the dynamics with details and he/she had possibility interrupting the calculations in order to change the parameters. The use of object-oriented approach has allowed us to reach high level of usability: a researcher could navigate through all the tasks smoothly and successfully.

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SEMBLANZA CURRICULAR

En 1975 estudio la Licenciatura y Maestría en la Universidad Nacional de Kiev (KNU), en la Facultad de Física y en el Departamento de Física Teórica. El Ph.D. (candidato en Ciencias físico - matemáticas) y el D.Sc. (Doctor en Ciencias físico matemáticas), los obtuvo también en la KNU en 1979 y 1988, respectivamente. Actualmente es Profesor-Investigador Titular “C” definitivo del Centro de Investigaciones en Ingeniería y Ciencias Aplicadas (CIICAp) de la Universidad Autónoma del estado de Morelos (UAEM), desde 1998. El Dr. Burlak es autor y coautor de cuatro libros y 116 artículos en revistas arbitradas. Ha participado en 118 ponencias en congresos nacionales e internacionales. Destaca su labor en la formación de recursos humanos, en los últimos tres años, ha dirigido 2 tesis de doctorado, 3 de maestría y 1 de licenciatura. Desde 2000 es miembro del Sistema Nacional de Investigadores, donde tiene el nivel II. Es miembro regular de la Academia de Ciencias de Morelos, de la American

Physical Society (1994 - a la fecha). Se desempeñó también como Arbitro del CONACyT de proyectos de Investigación Científica Básica y como Referee de las revistas internacionales “Physics Letters A”;“ Physica-D”.

LINEAS DE INVESTIGACION

• Las investigaciones de multicapas micro esféricas, optimización de los parámetros electromagnéticos y radiación óptica de micro-esferas activas cubiertas.
• Óptica cuántica. Emisión espontanea. Entanglement.
• Los problemas de interacciones de ondas no-lineales en solidos limitados, fibras, guías de ondas de la óptica integrada, formacion de estructuras disipativas. Dinámica no lineal del Bose-Einstein condensate.