Computer simulation of the optical radiation from coated microsphere with active core

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Abstract: - We have studied numerically the regimes of optical radiation from a coated microsphere with a gain substrate (active core). We found that the reflection coefficient can exceed unit in the band of gain. The Q factor of complex eigenfrequencies inside of gain area can become negative when number of layers in the stack is large enough. Threshold of generation is optimal for the dipole mode radiation.

Key-Words: - Electromagnetic waves, microsphere, multilayered stack, active core, computer simulation

1 Introduction

Nowadays the essential progress in technology of creation of dielectric microspheres with the sizes about ***0.1-20mm*** was achieved. It allows to pass to a new level of integration of devices of optoelectronics with using of microspheres as one of important controlling elements. Recently, the fabrication and optical properties of different kinds of microcavities which contain semiconductor nanoclusters or quantum dots (QD) was achieved (see [1-4] and references therein]. When semiconductor QDs are embedded in the spherical microcavity, the QD luminescence can couple with the eigen electromagnetic modes of microcavity and a lower threshold of stimulated emission (or lasing modes) of QDs may be realized. In [2-5] the coupling between the optical emission of embedded $CdSe_xS_{1-x}$, QDs and spherical cavity modes was investigated. The strong whispering gallery mode resonances with high Q factors are registered in the photoluminescence spectra.

Up to now modes with small numbers of spherical harmonics (SNM) are investigated weakly compare with WGM because of their rather low Q-factor caused by significant radiating losses. The principal opportunity of the sharp increase of Q factor of such oscillations was offered in a number of works [5-7]. The idea consists in coating of microsphere by alternative layers of a spherical stack. As a result it is possible to increase Q factor up to values, compare for WGM i.e. 10^7-10^9. Already while number of layers is about ***10*** it is possible to achieve Q factor about 10^6-

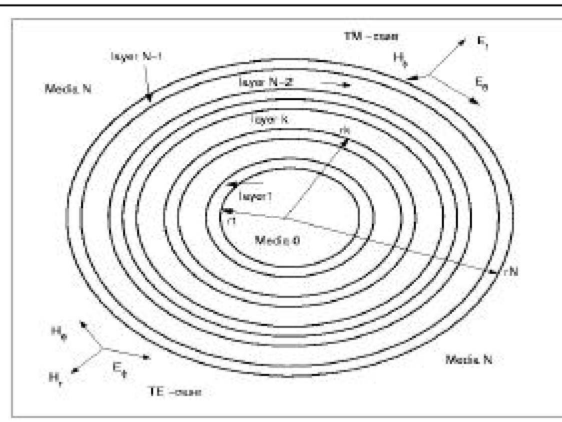

Fig. 1. Geometry of layered system

10^8. Moreover, using of the materials with strong frequency dispersion in the stack allows for SNM to achieve ***Q*** factor about 10^9 in infrared (IR) range if the dielectric permittivity becomes negative for some layers in a stack [8]. At the same time from the point of view of effective coupling with the active substrate SNM are rather attractive.

These modes are more deeply located in the substrate. For first dipole mode the maximum of the electric component of the optical field is located in the center of the core [9,10]. While the wave process in core consists of superposition of the re-reflected waves, such modes have time to interact with the active substrate more effectively, before to be radiated in the surrounding medium.

2. Basic equations

We consider a dielectric microsphere and a periodic system of multilayers deposited on it (see Fig.1). We assume here a microsphere with active core coated by a stack of dielectric alternating layers. In substrate and layers the set of Maxwell's equation is

$$\nabla \times \vec{E} = -iwm_0 \vec{H}, \nabla \times \vec{H} = iwe_0 e(w) \vec{E} \qquad (1)$$

Where $\vec{E}, \vec{H}$ are electrical and magnetic field, and ***e(w)*** is a complex dielectric permittivity. We use the complex exponential multiplier in form ***exp(iwt)***. We assume, that in a glass substrate is implemented the semiconductor with system of quantum dots, similarly to experiment [2].

We use the simplest phenomenological model of a QD considering exciton as a Lorentzian contribution to the dielectric constant e_h of the QD material (see, e.g., [11]) and restricting ourselves to the single-resonance approximation.

$$e(w) = e_h - \frac{2g_0 w_0}{w^2 - w_0^2 - i2wn}, \qquad (2)$$

where w_0 is the exciton resonant frequency; $n = 1/t$, t is the exciton lifetime. Near to a resonance $w \approx w_0$ the dielectric permittivity becomes a well-known form

$$e(w) = e_h - \frac{g_0}{w - w_0 - in} \qquad (3)$$

In equation (3) the parameter g_0 is related to the oscillator strength per dot. The dielectric permittivity of a host material e_h is assumed frequency independent. The case $g_0 > 0$ corresponds to QD with inverted population of levels, thus characterizing optical gain. Outside of band of the resonance at $\omega \neq \omega_0$ the dielectric permittivity ***e(w)*** is practically constant and equal to ε_h.

System (1) in the spherical coordinate frame (r, j, q), we reduce to Helmholz equation for a scalar function called a Debye potential.

We should join the solution for fields on boundaries of neighboring layers using standard conditions of continuity of fields. The method of calculation is based on a transverse matrix approach generalized to a spherical geometry [8]. We apply it to the case of a spherical stack with dielectric layers and the active core having material dispersion (2). In every layer of the stack one uses the next matrix presentation for fields:

$$\vec{u} = \begin{bmatrix} H_j \\ E_q \end{bmatrix} = \overleftrightarrow{D} \cdot \begin{bmatrix} a \\ b \end{bmatrix}, \qquad (4)$$

Where ***a*** and ***b*** are arbitrary constants, matrix $\overleftrightarrow{D} = \overleftrightarrow{D}(y)$ is written in [9,10], $y = wn(w)r/c$, $n(w) = [e(w)]^{1/2}$ is the refractive index of a particular layer of the stack.

This relation can be rewritten for a general case as follows. Let's start from the bottom layer of the stack with number ***k=1***. Using the recursive procedure we can write down

$$\vec{u}_1 = \overleftrightarrow{M}_2 \vec{u}_2 = \ldots = \overleftrightarrow{M} \vec{u}_N, \qquad (5)$$

Where

$$\overleftrightarrow{M} = \prod_{k=1}^{N-1} \overleftrightarrow{M}_k \qquad (6)$$

is the transfer matrix between inner (***k=1***) and outer (***k=N-1***) layers in the spherical stack. We have used Sommerfeld's radiation conditions, there is only the outgoing wave at the external boundary. As a result one readily obtains the coefficients of reflection ***R*** and transmittance ***T*** in form

$$R = \frac{Q_{21}(w)}{Q_{11}(w)}, T = \frac{1}{Q_{11}(w)} \qquad (7)$$

We suppose the absence of singularity in the center of core $r \rightarrow 0$. In result we obtain the eigenfrequencies equation in closed form

$$\Delta(n(w), w) = Q_{21}(w) - Q_{11}(w) = 0, \qquad (8)$$

Where

$$Q = (D_0)^{-1} \cdot M \cdot D_N \qquad (9)$$

where both the material and geometric dispersion is taken into account. Further we apply the above-developed theory to calculate the reflectance, transmittance, eigenfrequencies and eigen fields for the active microsphere with multilayered spherical dielectric stack.

3 Results and discussion

The following parameters have been used in calculations: the geometry of a system is ***SLNLNLN..NV*** where letters ***S,L,N,V*** indicate the materials in the $l/4$ stack, the radius of the active core (internal substrate is $r_1=16$mm . We have used the parameters of materials S (internal substrate): glass ***n=1.5*** **,** ***L:*** SiO_2**,** the thickness ***0.3mm*** **,** ***n=1.46*** , for calculations we used $t = 1.6 \times 10^{-12} sec^{-1}$, ***N: Si*** the thickness ***0.122mm, n=3.58***, ***V*** (outer medium): air, ***n=1***. The number of the spherical harmonic ***m=1***, or ***2***. We follow a simple estimate $g_0 = 10^{14} sec^{-1}$ and less[12].

The first question, which we are interesting to is how sufficiently is the influences of both dispersion and gain in the internal substrate to the reflection

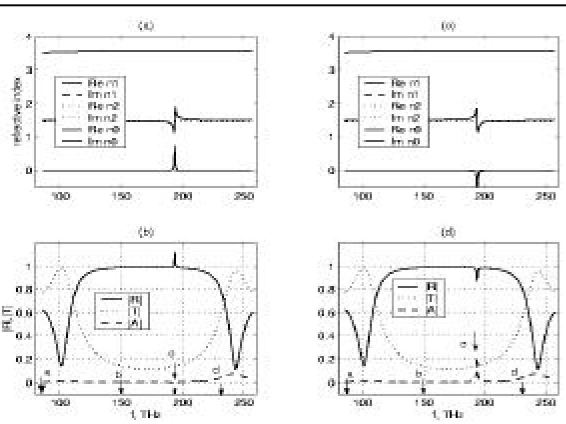

Fig.2. (a) Real and imaginary parts of refraction indexes substrate, layers of stack and gain factors.

coefficient in such the system. In Fig.2 the frequency dependence of refraction indexes of the internal substrate and layers of the stack for cases of amplification $g_0>0$ (a) and absorption $g_0<0$ (c) accordingly is shown. Total dielectric permittivity of such substrate looks like (2). In Fig.2(a and c) we use $g_0=2.6 \times 10^{12} sec^{-1}$. In Fig.2(b,d) the appropriate coefficients of reflection |***R***| and transmittance |***T***|, and

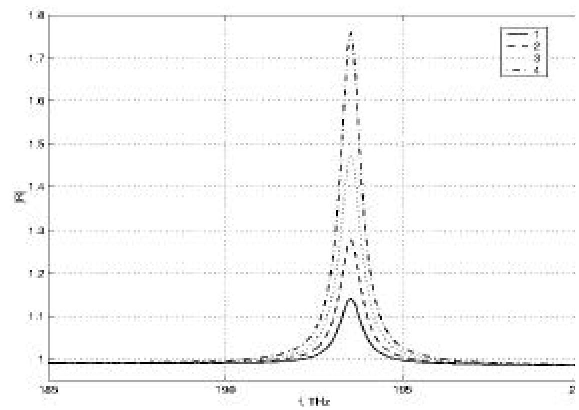

Fig.3. The frequency dependence of mofulo of the reflection coefficient |R| for different levels of the

also coefficient of losses $A=1-|R|^2-|T|^2$ are shown. One can see arising of the narrow peak (in a gain case) and of the hollow (in case of absorption) in the vicinity of the exciton resonance on the reflection's curve. The losses coefficient ***A*** becomes negative in the gain band that corresponds to the regime of generation in microsphere.

In Fig.3 the details of the frequency dependence of reflection coefficient are shown for several values of the gain factor g_0. One can see, that in the band of a resonance |***R***| sharply grows and for $g_0=6 \times 10^{12}$ sec^{-1}

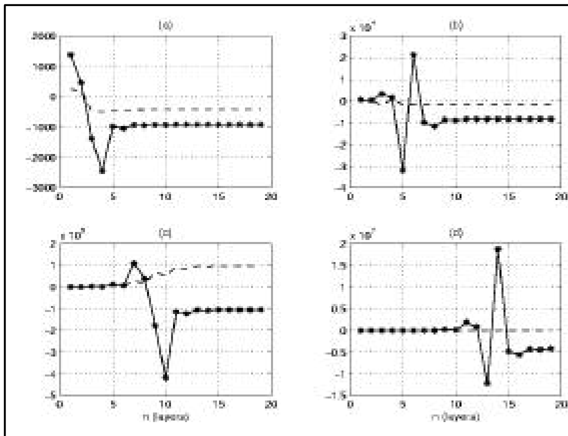

Fig.4. ***Q*** factors of eigenfrequency ***f=193.5*** THz within a gain-band versus number of layers in the stack ***n*** for the various gain factors g_0.

the |***R***| exceeds unit on ***80%***. At the same time the transmittance |***T***| varies a little bit only in the zone of the resonance (see Fig.2(b, d)). It is due to that the gain environment is beyond of the stack and it can not change the transmittance properties of the stack.

To elucidate the influence of structure of the coated microsphere on a regime of generation we have calculated a few representative eigenfrequencies, as inside of the gain zone, and also beyond of it. Such complex eigenfrequencies were calculated by the solving of the eigenfrequencies equation (8). We have studied the influence of number of layers in the stack both on real and image parts of eigenfrequencies. We analyze four eigenfrequencies (see. Table 1 and also Fig.2(b,d)). Note that frequency f_c is inside of the band-gain resonance, and frequency f_b is in the zone of strong reflection.

No	a	b	c	d
Re f, THz	85	150	193.5	231

Table 1. Some eigenfrequencies around of the band-gain of the active coated microsphere.

Further we use frequency $f=w/2p$ instead of w. In Fig.4 the dependence of Q-factor ($Q = Re(w)/2Im(w)$) of eigenfrequencies from ***Table 1*** vs number of layers at various levels for gain-factor g_0 are shown. In Fig.4 the Q factor of eigenfrequency inside of the band-gain f_c=***193.5TGz*** (l=***1.55mm***) is presented. One can see from Fig.4, while number of layers in stack is small the Q factor is positive and system does not generate. It corresponds to a case when the radiative losses of optical oscillations to the surrounding medium are substantial. However with increasing of number of layers in the stack Q factor changes the sign and becomes negative (i.e. changes the sign of $Im(f)$). Due to of the exponential factor $exp(iwt)$ it means the transition of system to the regime of generation of oscillation frequency f_c . One can see that the threshold's number of layers increases while reduction of the gain factor g_0. Indeed to achieve the generation for $g_0=7.78 \times 10^7$ sec^{-1} it is necessary to get $l/4$ stack with ***12*** layers. For our parameters at $g_0 = 4.34 \times 10^{11}$ sec^{-1} and less the change of the sign Q was not observed at all. In case of $g_0 > 5 \times 10^{13}$ sec^{-1} and more the Q becomes negative for any number of layers in the stack.

Thus in the overcritical regime the generation of the optical radiation with eigenfrequencies in the gain-band can be achieved when the number of layers in the stack is large enough. The radial distribution of the optical field of such eigenfrequency is of interest. We have calculated such the dependence for different number of layers in the stack. In the active core $r < r_1$ the structure of the field practically does not change above or below the threshold. However the amplitude of the optical field in external boundary of the stack $r > r_1$ varies substantially while changes the number of layers.

We found, that the threshold of generation of the optical eigenfield with number of the spherical harmonic $m=2$ exceeds the threshold for the dipole case $m=1$ approximately on one order of magnitude.

We believe, that it is owing by the radial structure of such eigenmodes: only $m=1$ mode has maximal value of electric field in the center of sphere $r=0$ [10,11]. For higher modes the eigenfield equal zero in the center of microsphere. Consequently the dipole radiation has optimal overlapping for coupling with the active substrate. We note also that such effect provides the opportunity to use the coated microspheres for effective harmonic generation in the optical range [13,14]. Also an important direction is using the microspheres for the change of the spontaneous emission of radiation (see [15] and references therein).

4. Method of calculation

For our calculation we use a object-oriented approach in system Borland C++ Builder. According hierarchy of classes is shown in Fig.5. The form of GUI is shown in Fig.6. We briefly describe such hierarchy structure in Fig.5.

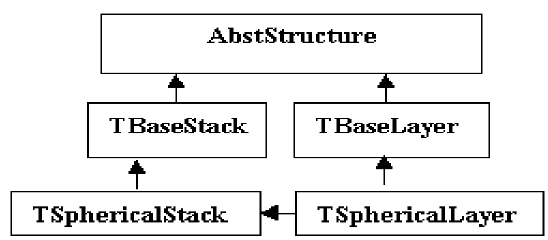

Fig.5. Hierarchy of classes

The base class AbstStructure includes the fields and all general abstract methods are necessary for definition of such a structure, as a spherical stack, and also as a dielectric layer. In classes-successors TBaseStack and TBaseLayer other additional members are accumulated, such members are responsible for the structure of the stack and layer. In a start of work the materials of the substrate and layers, the number of layers, and also the general type of the stack are assigned. For instance, there are a quarter-wave or half-wave stack, the factor of periodicity of the stack, etc. After that the dynamic objects of layers of class TSphericalLayer will be created accordingly to the hierarchy shown on Fig.5. Such objects are collected to the dynamic list, which

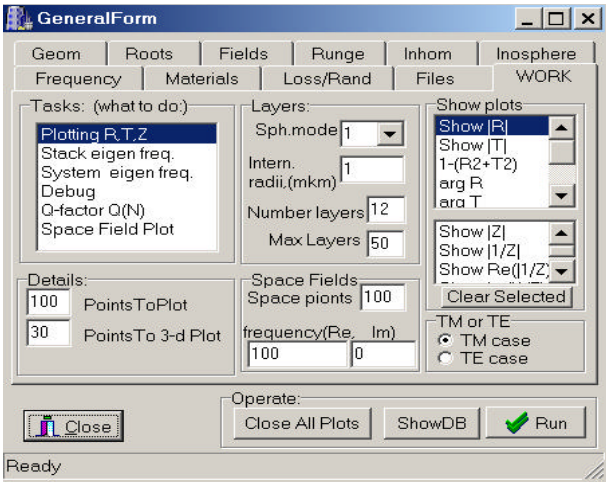

Fig.6. Graphic user interface for calculation of properties of spherical multilayered systems

itself is the object of class of spherical stack **TSphericalStack**. Since the stack is completed, one can perform the different types of jobs, which are listed in the Task menu, see Figs.6. For instance here are listed the jobs for calculation and plotting the coefficients of reflection and transmittance, calculation of complex eigenfrequencies and the radial distribution of eigenfields for given geometry, and also the calculation of dependence of ***Q***-factor of the stack versus the number of layers in the stack (see Fig.4).

5 Conclusion

We have studied regimes of optical radiation of compound system: active microsphere with the spherical stack deposited on it. It was supposed, that the internal spherical substrate has gain in a band of frequencies of the exciton resonance with lengthwave ***l=1.55mm***. By means of the matrix method we have derived the eigenfrequencies equation and analyzed some representative cases. Calculation shown, that in the gain regime the coefficient of reflection may exceed unit in the vicinity of the resonance. The ***Q*** factor of the eigenfrequencies being in the resonance zone may become negative when the number of layers in the stack is large enough. This occurs due to the compensation of the radiate losses by the gain of the optical field in the active substrate. In such regime the microsphere generates the optical radiation with spectrum of the eigenfrequencies inside of the gain-band. The threshold of generation is least in case of spherical harmonic ***m=1*** (dipole radiation). Let's note, that in [2,5] similar phenomenon was observed for microsphere (without stack) when spectrum optical WGM was registered. We have shown that such effect is rather sensitive to the structure of the spherical stack. This effect may find application in a number of active devices of optoelectronics. In such devices the selection of a few number of modes with opportunities of controlling by parameters of the optical field by means of electric, mechanical or other effects can be achieved.

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