POSSIBILITY OF APPLICATION OF THE NANOCOMPOSITES CONSISTING OF QUANTUM DOTS WITH THE PULSED LASER BEAM RADIATION IN NANOMEDICINE

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Abstract. *This paper discusses possibilities of using quantum dots in nanomedicine. The physical model is given, on the basis of which the relevant conclusions are made. The issue is equally important from both theoretical and practical points of view.*
Keywords: *nanoparticles, nanomaterials, nanomedicine, physical model.*

In recent years, there has been a significant increase in interest in the use of nanomaterials in medicine. However, it is important to identify number of fundamental topics as a result of relevant experiments, which will substantially clarify the possibility of practical application of quantum dots and other types of nanomaterials in nanomedicine.

As is well known, one of types of nanoparticles is quantum dots, which are a one-dimensional variety of nanoparticles. Based on results of theoretical studies, the possibility of application quantum dots in a nanomedicine is an important task today.

The quantum dots represent a heterostructure with spatial constraints in all three directions of charge transfer, which results in a substantial excess of energy between the electron levels and the significance of the thermal energy [1]. It should also be noted that this significant change and the ability to manage the energy spectrum at the expense of changes in the geometric size and shape of the quantum dot proved crucial to their practical application. However, the widespread use of quantum dots is hampered by the difficulty of obtaining them.

The paper discusses the possibility of application of the nanocomposites consisting of quantum dots with the pulsed laser beam irradiation for practical purposes. The appropriate physical model is proposed, on the basis of which appropriate conclusions are made. The issue under discussion has become more topical in recent years, which has increased interest in it. However, some aspects of the issue discussed here still require clarification in both theoretical and practical terms.

Theoretical model

As it is known, the maximum zone r_g, of quantum points islets up to which it can be increased in the process of the dislocation growth mechanism, is determined by the condition [2]:

$$\frac{d}{dr} = \left(\frac{\dot{r}}{r}\right)\Big|_{r=r_g} = 0, \quad (1)$$

from where do we get

$$\vec{r}_g = \frac{4}{3}\vec{r}_k; \quad (2)$$

where:

$\vec{r}_k$ - is the critical radius; and

$\dot{r} \equiv \frac{dr}{dt}$. - is a function of the distribution of specks by size, which we can write as follows [3]:

$$f(\vec{r}, t) = \varphi(\vec{r}_g) g(u), \quad (3)$$

$g(u)$ - is the distribution of specks according to relative dimensions $u = \frac{\vec{r}}{\vec{r}_g}$. in the equation (3).

$\varphi(\vec{r}_g)$ - can be determined from the law of mass storage of specks condensate

$$M = k \int_0^{r_g} r^2 f(\vec{r}, t) d\vec{r}, \quad (4)$$

where:

$k = \pi h\rho,\ \rho$ - is the density of the speck matter.

if we insert equation (3) in to equation (4), we get:

$$\varphi(\vec{r}_g) = \frac{Q}{r_g^3}; \qquad (5)$$

where:

$$Q = \frac{M}{k\int_0^1 u^2 du}.$$

to determine the $g(u)$ we can use the continuity equation

$$\frac{\partial}{\partial t}(f(\vec{r},t) + (f(\vec{r},t)\cdot\vec{r})) = 0. \qquad (6)$$

if in formula (6), instead $f(\vec{r},t)$ and $\dot{r}$ we enter their values and switch from r and t differentiation to u differentiation, then in formula (6) the variables will be separated and will take the form:

$$\frac{dg(u)}{g(u)} = -\frac{3\theta_g + 3\frac{\theta}{u^4} - \frac{1}{u^3}\frac{d\theta}{du}}{u\theta_g - \frac{\theta}{u^3}} du, \qquad (7)$$

Where it is provided that $\frac{dr_g}{dt} = \theta_g \frac{A}{r_g^3}$; $\frac{du}{dr_g} = -\frac{u}{r_g}$; $\theta = \frac{\dot{r}\cdot r^3}{A}$; $A = \frac{zC_\infty \sigma v_n^2 D_s^{(d)}}{kTln(l)}\sqrt{\frac{2q}{\pi}}$;

where:

r_k - is the critical radius;
k - is the Boltzmann constant;
T - is the temperature;
σ - is the surface energy;
C_∞ - is the equilibrium concentration at the speck boundary;
l - is the so-called "Screen distance"

$$(C(R) = \langle C\rangle|_{R=ir},$$

where:

$l = 2$ or $l = 3$) - Is the concentration of atoms at a distance R from the center of the speck,

$$C(R) = \frac{\langle C\rangle - C'}{\ln(l)}\cdot ln\frac{R}{r} + C',$$

where:

$\langle C\rangle$ - is the average concentration of atoms in the base layer;
C' - is the concentration of the substance on the surface of the speck.

Integrating of the (7) equation will give:

$$g(u) = \frac{u^3\exp\left(-\frac{1}{3(1-u)}\right)exp\left(-\frac{1}{9\sqrt{2}}arctg\left(\frac{u+1}{\sqrt{2}}\right)\right)}{(1-u)^{\frac{25}{9}}\cdot(u^2+2u+3)^{\frac{29}{18}}}. \qquad (8)$$

It is known that an acoustic-thermal effect can occur in the zone of biofiber irradiation with a laser beam. The result is a bifurcated area that can be described according to the methodology discussed in the paper [4]. In particular, in the above paper, to solve this issue, Newton's task is taken so-called inverse distribution function through which a bifurcation area can be described. In particular, it has been shown that the equation for Newton's problem has the form (9).

Let us now consider the above-mentioned waveguide environments in which the laser beam can propagate. Also consider the acoustic effects generated by the impact of the laser beam.

The study of the self-organization of quantum dots is highly relevant in terms of the use of nanotechnologies. To obtain structures with given properties it is necessary to be able to manage quantum dots according to size and density. Nanoclasts are currently being modified directly during the growth process. Technologically, laser radiation is mainly used during these processes.

In order to determine the temperature regime of a quantum dot, it is necessary to perform numerical modeling of the laser impact. If we neglect the absorption of laser radiation by nanoclasts, then we can limit it to a one-dimensional approximation because the intensity of the laser radiation is evenly distributed over the irradiated zone and its size is several times the length of the thermal diffusion. It is even a number of times longer than the duration of the pulse heating. The one-dimensional nonlinear heat conduction equation will have the form of Stephan's conditional phase transition boundary [5]:

$$\rho(x,T)[c(x,T)+L\delta(T-T_m)]\frac{\partial T}{\partial t}=\frac{\partial}{\partial x}\left[k(x,T)\frac{\partial T}{\partial x}\right]+Q(x,t);(11)$$

$$\left.\frac{\partial T}{\partial x}\right|_{x=0}=0,$$
$$T|_{x=D}=T|_{t=0}=T_0;$$

where:
T - is the temperature;
$T_0 = 300K,$ - is t-time,
x - coordinate is directed inside the sample;
ρ - is the density;
c - is the specific heat capacity;
k - is the thermal conductivity;
L - is the heat of complete melting;
T_m - is the melting temperature;
$\delta(T)$ - is a function of Dirac;
$Q(x,t)$ - function describes the release of heat during the absorption of laser radiation:

$$Q(x,t)=\alpha(T)(1-R)q(t)exp\left\{-\int_0^x \alpha[T(x')]dx'\right\};\quad (12)$$

where:
α - is the absorption coefficient;
R - is the reflection coefficient;
$q(t)$ - is the laser pulse shape and has the following form:

$$q(t)=\frac{W}{\tau_p}sin^2\left(\frac{\pi t}{2\tau_p}\right).\qquad (13)$$

When studying a particular substance it is necessary to take into account the temperature dependence of the optical and thermal parameters, as well as their dependence on the phase state. δ-function in the equation for the limit mode is necessary to determine the melting point of a monocrystal.

It is known that it is difficult to calculate the individual physical properties of a particular nanoparticle as a system because it is composed of many particles that conform to the laws of quantum mechanics. It is also known that the optical properties of a quantum mechanical system are related to the properties of the energy state spectrum of charge carriers: electrons and holes. To date, it can be established that the optical and electrophysical properties of nanoparticles differ significantly from properties of the bulk sample due to changes in their energy spectrum [6-9].

Analysis results

According to the mathematical model presented in the paper, optical-acoustic and thermo-acoustic effects occur in biofiber during quantum dot laser radiation. Consideration of these effects in this case is solved by the Newton's problem using the so-called inverse distribution function.

It can be seen from equation (5) that the magnitude of the light conduction coefficient in a dielectric nanocomposite is essentially dependent on the intensity of the laser radiation field (I). In particular, this dependence has a minimum point (I_p), in which the conduction coefficient is minimal for certain parameters of the composite and radiation. However, when shifting from the value of I_p to the large or small side, the effect of limiting the small radiation appears according to the intensity scale. The conduction spectrum profile is generally asymmetric with respect to the central frequency due to the difference in the $\Delta\omega_1$ and $\Delta\omega_2$ frequencies.

In the paper [12] equations of nanocomposites are given, from which it can be seen that the depth of the absorption band strongly depends on the magnitude of the intensity and the size of the nanoparticles. However, for solid dielectric nanocomposites, the orientation of the nanoparticle along the field requires a high intensity of radiation. It should also be noted that the conductivity coefficients for solid and liquid matrices are the same at high intensities. In this case, the value of the conduction coefficient to the central frequency is equal:

$$T(I)=\exp\left(-L\frac{4\pi\omega_n N}{c\hbar\Gamma_n}a^2(GS_n)_{g=n}(\Delta\omega_1+\Delta\omega_2)\cdot F^2(I)\right).$$

As the intensity increases, this equation exponentially tends to one, the faster the larger the nanoparticle size, $\Delta\omega_1 + \Delta\omega_2$, also the value of the GS.

Conclusion

Thus, the task under the model is solved based on the methodology presented in the paper [4]. This promotes a number of subtle effects to occur when a quantum dot is inserted into a biofiber and radiated laser beams. In this case, we consider the optical-acoustic and thermo-acoustic effects, which increases the accuracy of results obtained and simplifies the determination of the inverse distribution function of the source.

In particular, it follows from the equation, (18) that in a system in which the dipole-dipole interaction of the nanoparticle can no longer be neglected, the magnitude of this interaction will strongly depend on the intensity that will take the maximum value in the rather weak fields $(I \approx I_p)$. This peculiarity should be taken into account when studying the optical properties of similar composites, as well as when designing real devices whose work is based on this property.

It should be noted that studies conducted in the paper [5, 13, 14] found that the impact of a single pulse of a laser also changes properties of quantum dots, causing a partial relaxation of their size and composition. Even more substantial changes occur during exposure to 10 laser pulses.

As it is known, many materials of biological origin (proteins, bacteria) can be considered as nanoparticles, and at this time particles are dielectric. In this regard, the question arises about the existence of nonlinear low-threshold optical echoes in the biological environment, which is also no less interesting in terms of their practical application.

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ВОЗМОЖНОСТЬ ПРИМЕНЕНИЯ НАНОКОМПОЗИТОВ, СОСТОЯЩИХ ИЗ КВАНТОВЫХ ТОЧЕК, С ИМПУЛЬСНЫМ ЛАЗЕРНЫМ ИЗЛУЧЕНИЕМ В НАНОМЕДИЦИНЕ

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Аннотация. *В данной статье рассматриваются возможности использования квантовых точек в наномедицине. Дана физическая модель, на основе которой сделаны соответствующие выводы. Этот вопрос важен как с теоретической, так и с практической точек зрения.*

Ключевые слова: *наночастицы, наноматериалы, наномедицина, физическая модель.*