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Modeling the deformation of the semiconductor quantum dot with a multilayer shell in a living cell

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The model of the semiconductor quantum dot with a multilayer shell and the quantum dot-human serum albumin bionanocomplex, which are contained in a living cell, was constructed. The regularities of changes in deformation of materials of the CdSe-core / ZnS/CdS/ZnS-shell quantum dot with changes in cell elasticity (comprehensive modulus) at different core radii, thicknesses of individual shell layers, and surface concentration of albumin molecules were investigated. It is shown that the presence of human serum albumin on the surface of the quantum dot significantly increases its sensitivity to pressure caused by the surrounding medium (living cell). The obtained results indicate the prospect of using the core-shell quantum dot-human serum albumin bionanocomplexes for the diagnosis of cancer diseases in the early stages. This is due to the fact that such diseases are accompanied by a sharp change in the elasticity of the cell (its elastic constants).

Keywords: core-shell quantum dot, human serum albumin, deformation, comprehensive compression modulus, living cell.

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Introduction

Cancer progression is associated with changes in the cytoskeletal architecture of cells and thus in their mechanical properties, such as stiffness. Changes in cell mechanics allow cancer cells to migrate and invade distant organs. This process, metastasis, is a major cause of cancer mortality [1]. According to the most common results on the mechanics of different types of cancer, softness is a prominent characteristic of cancer cells, and its degree can give an estimate of cancer migration and invasiveness [2].

For example, it has been reported that the metastatic activity of human breast cancer cells can be increased by reducing cell stiffness [3, 4]. The results obtained in [5] showed that the actin organization of malignant thyroid cells is disrupted, giving malignant cells a two to five times lower Young's modulus compared to primary normal cells of the thyroid gland. Although in some works [6-9] it is shown, on the contrary, that the elastic constants of the diseased cells increase.

An analysis of the literature shows that for liquid-like cancer cells, which are softer than normal cells, the stiffness index is negative (elastic constants decrease), and for solid cancer cells, which are stiffer than normal cells, the stiffness index is positive (elastic constants increase).

In works [10, 11], it was established that cancer cells already at an early stage reduce their elasticity, change the value of the elastic constants. This fact can be used to diagnose disease using quantum dots (QDs) that are sensitive to deformation.

Semiconductor QDs have a wide absorption spectrum, narrow emission spectrum, large Stokes shift, high quantum yield and photostability, significant sensitivity and biocompatibility [12-14]. Therefore, QDs have prospects for use in nanobiology and nanomedicine, in particular, they can be used as fluorescent labels to control the targeted delivery of drugs in real time or to monitor the treatment of malignant tumors. The CdSe QDs are widely used in this area. But QDs have a high density of surface defects (due to the high ratio of surface area to volume), that act as centers of non-radiative recombination of carriers in QDs. This leads to a decrease in the intensity of photoluminescence due to the transfer

of electric charge from the QD to the molecule of the anticancer drug. One method of solving this problem is to create quantum dots with a protective shell that contains one or more layers. Therefore, CdSe QDs, which have a multicomponent structure of the shell (ZnS/CdS/ZnS), at a small thickness, passivate much better the reduction of the QD photoluminescence quantum yield, compared to both thin and thick ZnS shells. Such QDs can become optimal fluorescent labels for the creation systems of diagnosis and treatment of cancer. Mechanical deformation is an important factor that affects the optical and electrical properties of QDs with a multilayer shell. Cancer cells absorb quantum dots more actively than healthy cells. This is due to a change in the elasticity of the surrounding medium, namely, a change in elastic constants. All this should be reflected in the change in mechanical strain and deformation of the QD, and the established regularities of the change in the spectral composition of the radiation of the fluorescent label based on the QD will make it possible to assess the stage of the disease. The deformation of the QD leads to a local shift of the edges of the allowed bands, and this, in turn, leads to a change in the energy spectrum of electrons and holes and, accordingly, the optical properties of the QD. Thus, establishing the regularities of changes in the deformation of CdSe QDs with a multicomponent shell when changing the elastic constants of the cell (cytoplasm or core) is an urgent task in the context of their use in medicine.

One of the directions of research of QDs for their biomedical applications is the study of their interaction with proteins, in particular with human serum albumin (HSA) [13, 15-17]. The addition of human serum albumin to the colloidal solution of nanoparticles leads to a decrease in the optical density and a blurring of the exciton structure in the absorption spectra [15, 16]. This behavior indicates the interaction of semiconductor nanoparticles with HSA with the formation of appropriate biocomplexes.

In this work, the model of the QD with a multilayer shell and its bionanocomplex with HSA, which undergoes deformation under the influence of the elastic medium of the cell of the biological object into which it enters, is constructed.

I. The model

Let's consider the QD with a multilayer shell (QD-HSA bionanocomplex) as an elastic dilatational inclusion in the elastic medium of the cytoplasm or core of a living cell (Fig. 1). The spherical CdSe / ZnS/CdS/ZnS QD with a three-layer shell with core radius R_0 and thicknesses of the i-th layer of the shell $d_i = R_i - R_{i-1}$ (i =1, 2, 3) is considered. QD, due to the non-zero volume V, deforms the living cell, creating a mechanical strain $\sigma = -K\,V/V_0$, where K is the module of comprehensive compression of the cell; V_0 is the volume of the cell per one QD. As a result, the deformed elastic medium of the cell creates pressure on the QD surface:

$$P_c = -\sigma = KV/V_0. \qquad (1)$$

The volume of the QD with a three-layer shell: $V = \frac{4}{3}\pi R_3^3$, where R_3 is the radius of the outer layer of the shell.

The volume of the QD with a three-layer shell–HSA bionanocomplex: $V = \frac{4}{3}\pi(R_3 + d_\alpha)^3$, where d_a is the thickness of the HSA layer.

To determine the components of the deformation tensor, it is necessary to find an explicit form of the displacements of atoms $u_\gamma^{(i)}$ in the materials of the QD core (i = 0) and the shell layers (i = 1, 2, 3) [18, 19]. To this end, we write down the equation of equilibrium

$$\vec{\nabla} div\,\vec{u} = 0 \qquad (2)$$

with the following boundary conditions:

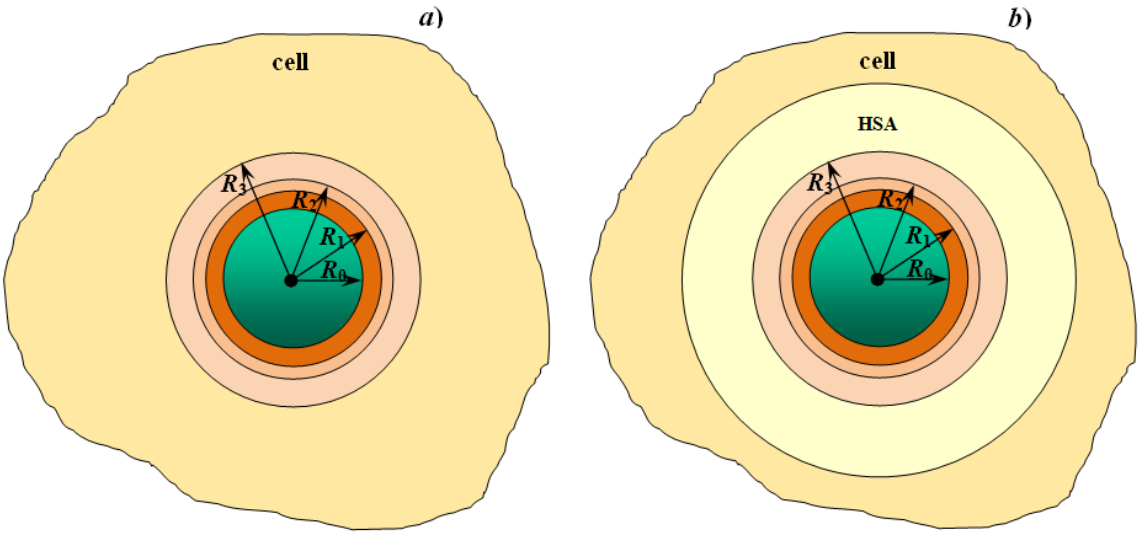

Fig. 1. The model of the spherical QD of the core-three-layer shell type (a) and the QD–HAS bionanocomplex (b), which are located in a living cell.

$$\begin{cases} 4\pi R_0^2\left(u_r^{(i+1)}\big|_{r=R_i} - u_r^{(i)}\big|_{r=R_i}\right) = \Delta V^{(i)}, \\ \sigma_{rr}^{(i)}\big|_{r=R_i} + P_L^{(i)}(R_i) = \sigma_{rr}^{(i+1)}\big|_{r=R_i} + P_L^{(i+1)}(R_i), \quad i = 0,1,2, \\ \sigma_{rr}^{(3)}\big|_{r=R_3} + P_L^{(3)}(R_3) = -P_c - P_a; \end{cases} \tag{3}$$

where $\Delta V^{(i)} = f^{(i)} \cdot 4\pi(R_i^3 - R_{i-1}^3)$ is the change in the volume of QD in the vicinity of the corresponding heteroboundary due to the mismatch of lattice parameters $f^{(i)} \approx \frac{a^{(i+1)} - a^{(i)}}{a^{(i)}}$ ($a^{(i)}$ is the crystal lattice parameter) [18]; $P_L^{(i)}(R^i) = \frac{2\gamma^{(i)}}{R^i}$ is the Laplace pressure; $\gamma^{(i)} = \frac{\gamma_{bulk}^{(i)}}{1+\frac{2\delta}{R_i}}$ [20] is the surface energy of the core or the corresponding layers of the shell, the values of which for CdSe, ZnS, CdS nanoparticles were determined in works [21, 22]. The right part of the third equation determines the pressure from the elastically deformed cell P_c and the pressure due to the attraction of HSA molecules to the QD surface P_a (for the case of the QD–HSA bionanocomplex) [22]:

$$P_a = \frac{n_s}{1+n_s S_A} p \frac{dE}{dr}\Big|_{r=R_3} \tag{4}$$

where n_s is the surface concentration of HSA molecules; S_A is the effective cross section of HSA molecule, $S_A = 9 \cdot 10^{-14}\ cm^{-2}$; p is the dipole moment of the albumin molecule; R_3 is the radius of the outer layer of shell, E is the intensity of the electric field created by QD. In more detail, the procedure for determining the pressure created by human serum albumin on the QD surface is described in [22].

The mechanical strain $\sigma_{rr}^{(i)}$ in the core and the shell layers of QD is determined by the formula:

$$\sigma_{rr}^{(i)} = \frac{E_i}{(1+\nu_i)(1-2\nu_i)}\left[(1-\nu_i)\varepsilon_{rr}^{(i)} + \nu_i\left(\varepsilon_{\varphi\varphi}^{(i)} + \varepsilon_{\theta\theta}^{(i)}\right)\right] \tag{5}$$

Knowing the displacement, we determine the components of the deformation tensor of the materials of the core and the shell layers of QD:

$$\begin{gathered} \varepsilon_{rr}^{(i)} = \partial u_r^{(i)}/\partial r, \\ \varepsilon_{\varphi\varphi}^{(i)} = \varepsilon_{\theta\theta}^{(i)} = u_r^{(i)}/r, \\ \varepsilon^{(i)} = \varepsilon_{rr}^{(i)} + \varepsilon_{\theta\theta}^{(i)} + \varepsilon_{\varphi\varphi}^{(i)}. \end{gathered} \tag{6}$$

II. Calculation results and their discussion

In Fig. 2 shows the dependence of the deformation of the CdSe-core/ZnS/CdS/ZnS-shell QD materials on the value of the comprehensive compression modulus of the cell in the interval up to 0.2 MPa for different thicknesses of the inner layer of the ZnS shell at the core radius of R_0 =10 nm (the deformation of QD, which is not subjected to pressure from the cell, is taken as zero deformation). Such dependence has a linear character. The values of the modulus of elasticity for a healthy cell lie in the range (0.1-1) bar. Cytoplasm has lower values, cell core has higher values. In a diseased cell, these values may decrease (increase) several times. In case of decrease or increase in cell elasticity (depending on the disease), the amount of deformation of QD materials and, accordingly, the energy spectrum of QD radiation will change. The QD core is the most sensitive to changes in cell elasticity. An increase in the thickness of the shell leads to an increase in the compression deformation of all layers of the heterostructure.

The sensitivity of QD materials to changes in cell elasticity increases significantly when using QD–HSA biocomplex (Fig. 3). In this case, the character of the dependence of the deformation on the modulus of elasticity does not change, but the deformation of QD materials and its change with a change in the comprehensive compression modulus increases approximately 4-6 times depending on the surface concentration of albumin (Fig. 3a,b). This is due to the occurrence of additional pressure due to the electrostatic attraction of albumin molecules to QDs.

In Fig. 4 shows the dependence of the deformation of the CdSe-core/ZnS/CdS/ZnS-shell QD materials (Fig. 4a) and QD–HSA biocomplex (Fig. 4b) on the radius of the QD core, at a surface concentration of HSA of 10^{14} cm^{-2}. An increase in the radius of the QD core, as well as the thickness of the shell layers, leads to an increase in the compression deformation of all materials of the heterostructure. This is mainly due to an increase in the QD volume and, accordingly, an increase in the deformation of the cell itself, which exerts greater pressure in response. The inner layer of the CdS shell undergoes a slight compression deformation, which slowly increases (compared to other layers of the heterostructure) as the core radius increases. The presence of HSA molecules on the QD surface makes it significantly more sensitive to the deformation created by the pressure of the cell at any radii of the QD core.

In Fig. 5 shows the dependence of the deformation of the CdSe-core/ZnS/CdS/ZnS-shell QD materials on the surface concentration of HSA (R_0 = 10 nm) and different thicknesses of the shell layers. An increase in the concentration of albumin leads to an increase in the absolute value of the compression deformation of all materials of the nanostructure. But it should be noted that a significant increase in compressive deformation is observed for insignificant concentrations of HSA ($n_s < 0.6 \cdot 10^{14}$ cm^{-2}). With a further increase in the concentration of albumin, the QD deformation practically does not change. This is explained by the fact that a

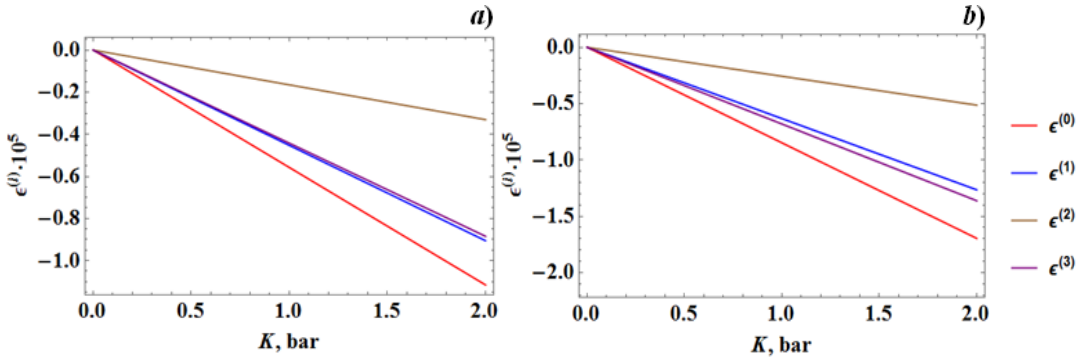

Fig. 2. The dependence of the deformation of the CdSe-core/ZnS/CdS/ZnS-shell QD materials on the value of the comprehensive compression modulus of the cell at the core radius of R_0 =10 nm and for the thickness of the shell layers: $d_1 = 2a^{(1)}$ (a); $d_2 = 2a^{(2)}$; $d_3 = 2a^{(3)}$; $d_1 = 6a^{(1)}$ (b)

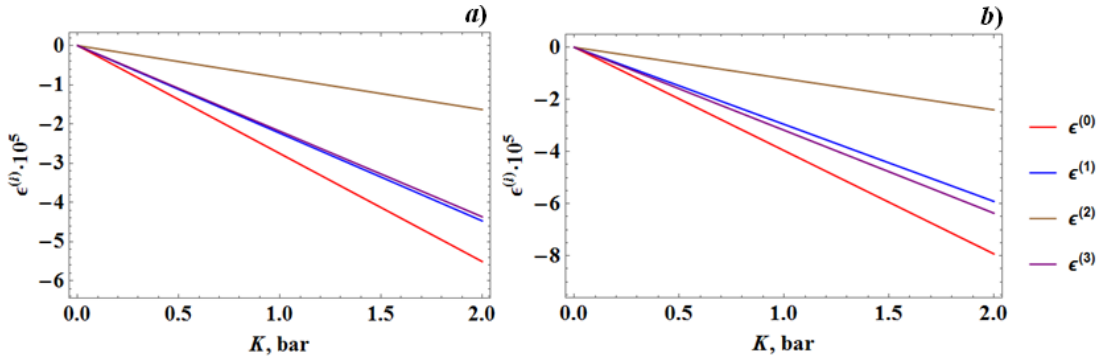

Fig. 3. The dependence of the deformation of the CdSe-core/ZnS/CdS/ZnS-shell QD materials on the value of the comprehensive compression modulus of the cell compression for the QD–HSA biocomplex at the surface concentration of $n_s = 10^{14}$ cm^{-2} and at the core radius of R_0 =10 nm for the thickness of the shell layers: $d_1 = 2a^{(1)}$ (a); $d_2 = 2a^{(2)}$; $d_3 = 2a^{(3)}$; $d_1 = 6a^{(1)}$ (b).

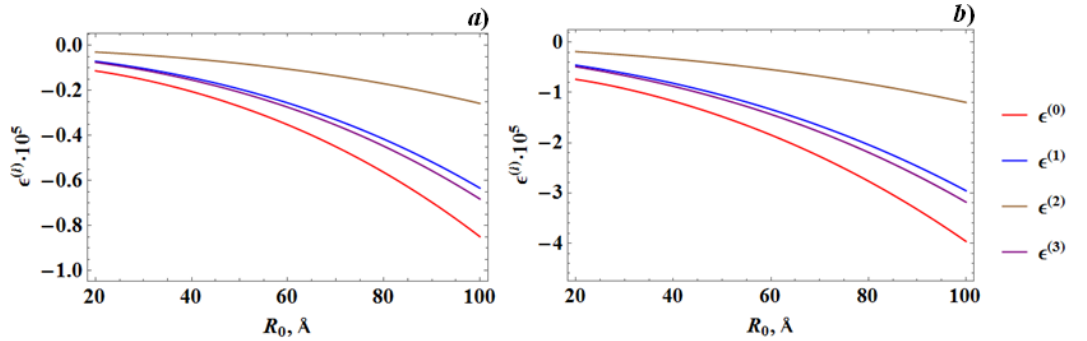

Fig. 4. The dependence of the deformation of the CdSe-core/ZnS/CdS/ZnS-shell QD materials (a) and QD–HSA biocomplex (b, $n_s = 10^{14}$ cm^{-2}) on the radius of the QD core for the thickness of the shell layers: $d_1 = 2a^{(1)}$ (a); $d_2=2a^{(2)}$; $d_3 = 2a^{(3)}$. Here K = 1 bar

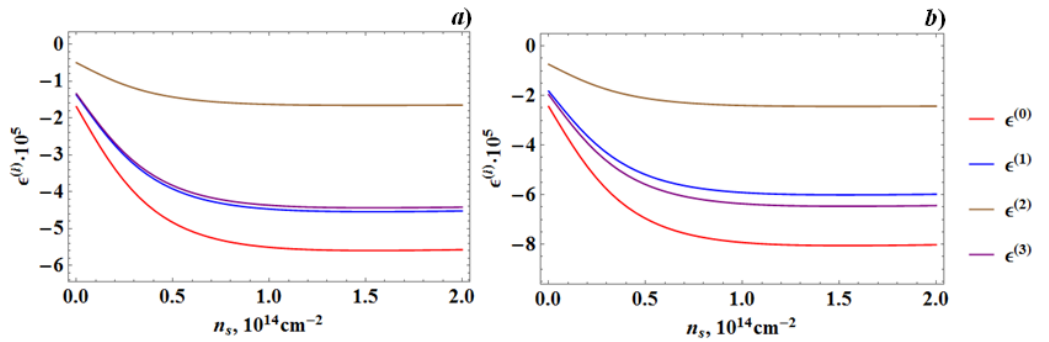

Fig. 5. The dependence of the deformation of the CdSe-core/ZnS/CdS/ZnS-shell QD materials on the surface concentration of HAS at the core radius of R_0 =10 nm and for the thickness of the shell layers: $d_1 = 2a^{(1)}$ (a); $d_2=2a^{(2)}$; $d_3 = 2a^{(3)}$; $d_1 = 6a^{(1)}$ (b)

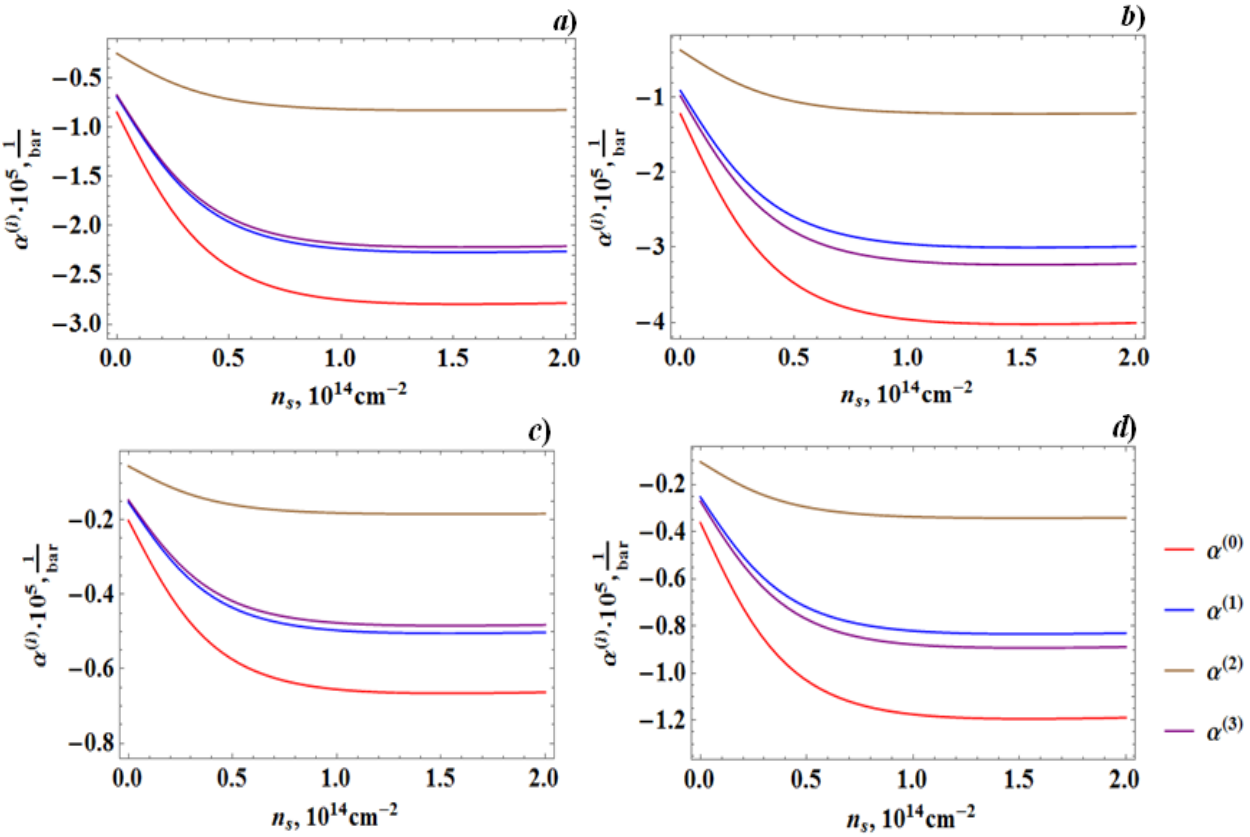

Fig. 6. The dependence of the parameter $\alpha^{(i)}$ of the CdSe-core/ZnS/CdS/ZnS-shell QD materials on the surface concentration of HSA at the core radii R_0 =10 nm (a, b) and R_0 =4 nm (c, d) for the thickness of the shell layers: $d_1=2a^{(1)}$ (a, c); $d_2 = 2a^{(2)}$; $d_3 = 2a^{(3)}$; $d_1 = 6a^{(1)}$ (b, d).

limited number of HSA molecules can interact with the QD surface. When using QDs for the diagnosis of cancer diseases, an important parameter is not only the absolute value of the deformation, but also the sensitivity of the deformation of the QD materials to changes in the elastic constants of the cell:

$$\alpha^{(i)} = d\varepsilon^{(I)}/dK$$

In Fig. 6 shows the dependence of the parameter $\alpha^{(i)}$ of the CdSe-core/ZnS/CdS/ZnS-shell QD materials on the surface concentration of HSA for different geometric sizes of the QD core and shell. An increase in the concentration of HSA molecules increases the sensitivity of nanoheterostructure materials to changes in the elasticity of a living cell. Depending on the core radius and the thickness of the shell, the presence of HSA on the QD surface allows to increase the parameter $\alpha^{(i)}$ by 3-3.5 times. Moreover, this parameter is the largest in absolute value for the CdSe core and the smallest for the CdS inner layer for any QD size and HSA concentration. Increasing the radius of the QD core and the thickness of the ZnS shell layers also increases the parameter $\alpha^{(i)}$. Thus, when the core radius changes from 4 nm (Fig. 6c) to 10 nm (Fig. 6a) at the HSA concentration $n_s = 0.5\cdot10^{14}$ cm^{-2}, the parameter $\alpha^{(0)}$ increases from $0.63\cdot10^{-5}$ 1/bar to $2.4\cdot10^{-5}$ 1/bar (almost 4 times). Increasing the thickness of the ZnS shell layer from $d_1 = 2a^{(1)}$ (Fig. 6a) to $d_1 = 6a^{(1)}$ (Fig. 6b) increases the parameter $\alpha^{(0)}$ by 50%. Changing the thickness of the inner layer of the shell practically does not change the deformation of QD materials and the parameter $\alpha^{(i)}$, which characterizes the sensitivity of QD to changes in cell elasticity.

Conclusions

The model of the core-three-layer shell QD and the QD-HSA bionanocomplex which are placed in a living cell was constructed. The proposed model considers the QD as an elastic dilatational inclusion, which is subjected to pressure from the cell depending on the comprehensive compression modulus.

On the basis of the developed model, the regularities of the change in deformation of the CdSe-core/ZnS/CdS/ZnS-shell QD materials when the elasticity of the cell changes depending on the geometric sizes of the QD and the surface concentration of human serum albumin have been established.

It was established that the CdSe/ZnS/CdS/ZnS – HSA bionanocomplex has greater sensitivity to changes in the elasticity of a living cell than the CdSe/ZnS/CdS/ZnS QD. This is explained by the occurrence of additional pressure on the QD surface due to the electron-deformation interaction.

It was established that QDs of larger sizes are more sensitive to changes in the elasticity of the cell in which they are located. This is mainly due to an increase in the QD volume and, accordingly, an increase in the deformation of the cell itself, which in response exerts greater pressure.

The obtained results indicate the prospect of diagnosing cancer diseases in the early stages with the help of the CdSe/ZnS/CdS/ZnS QDs and bionanocomplexes based on them. Already in the early stages, a diseased cell changes its elasticity (the value of elastic constants) by several times. This will affect the strained state of QDs and, accordingly, it will change the band structure, which should be reflected in the spectral characteristics of bionanocomplexes based on QDs.

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Моделювання деформації напівпровідникової квантової точки з багатошаровою оболонкою в живій клітині

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Побудовано модель напівпровідникової квантової точки з багатошаровою оболонкою та біонанокомплексу кантова точка – альбумін крові людини, які містяться в живій клітині. Досліджено закономірності зміни деформації матеріалів квантової точки ядро-CdSe/оболонка-ZnS/CdS/ZnS при зміні еластичності клітини (модуля всебічного стиску) за різних радіусів ядра, товщин окремих шарів оболонки та поверхневої концентрації молекул альбуміну. Показано, що наявність альбуміну крові людини на поверхні квантової точки суттєво збільшує її чутливість до тиску, спричиненого оточуючим середовищем (живою клітиною). Отримані результати свідчать про перспективу використання біонанокомплексів квантова точка виду ядро-оболонка – сироватковий альбумін крові людини для діагностики ракових захворювань на ранніх стадіях. Це пов'язано з тим, що такі захворювання супроводжуються різкою зміною еластичності клітини (її пружних сталих).

Ключові слова: квантова точка виду ядро-оболонка, альбумін крові людини, деформація, модуль всебічного стиску, жива клітина.