Acoustoelectronic effect in semiconductor quantum dots with a multilayer shell

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TOPICALITY and AIMS. An important factor that affects the spectral characteristics of radiation of the quantum dots (QDs) is elastic deformation. The source of elastic deformations can be both internal factors (the mismatch of lattice parameters, the point defects) and external factors. In particular, the cause of periodic deformation can be an acoustic wave. Such deformation can occur during electromagnetic irradiation of QDs. In this case, the thermo-deformation mechanism of sound generation is used. Also, the QDs are widely used in medicine and can be exposed to ultrasound.

QDs with a multi-layer shell also undergo significant deformations due to the mismatch of lattice parameters of the contacting layers. Therefore, there is a need to develop a model of the core-multilayer shell QD, that is exposed to an acoustic wave. As a result of the interaction of the acoustic wave with the electronic subsystem of the QD, the following effects can be observed: the periodic deformation due to self-consistent electron-deformation coupling leads to a local periodic displacement of the bottom of the conduction band and the top of the valence band and, accordingly, to the modulation of the energy of electron and hole and the width of the band gap; the emergence of a gradient of the refractive index under the influence of ultrasound leads to a periodic change in the direction of QD radiation;

the propagation of an acoustic wave in a certain direction leads to an increase in the size of QDs in this direction, and, accordingly, to a distortion of their shape and a change in the energy of electron and hole.

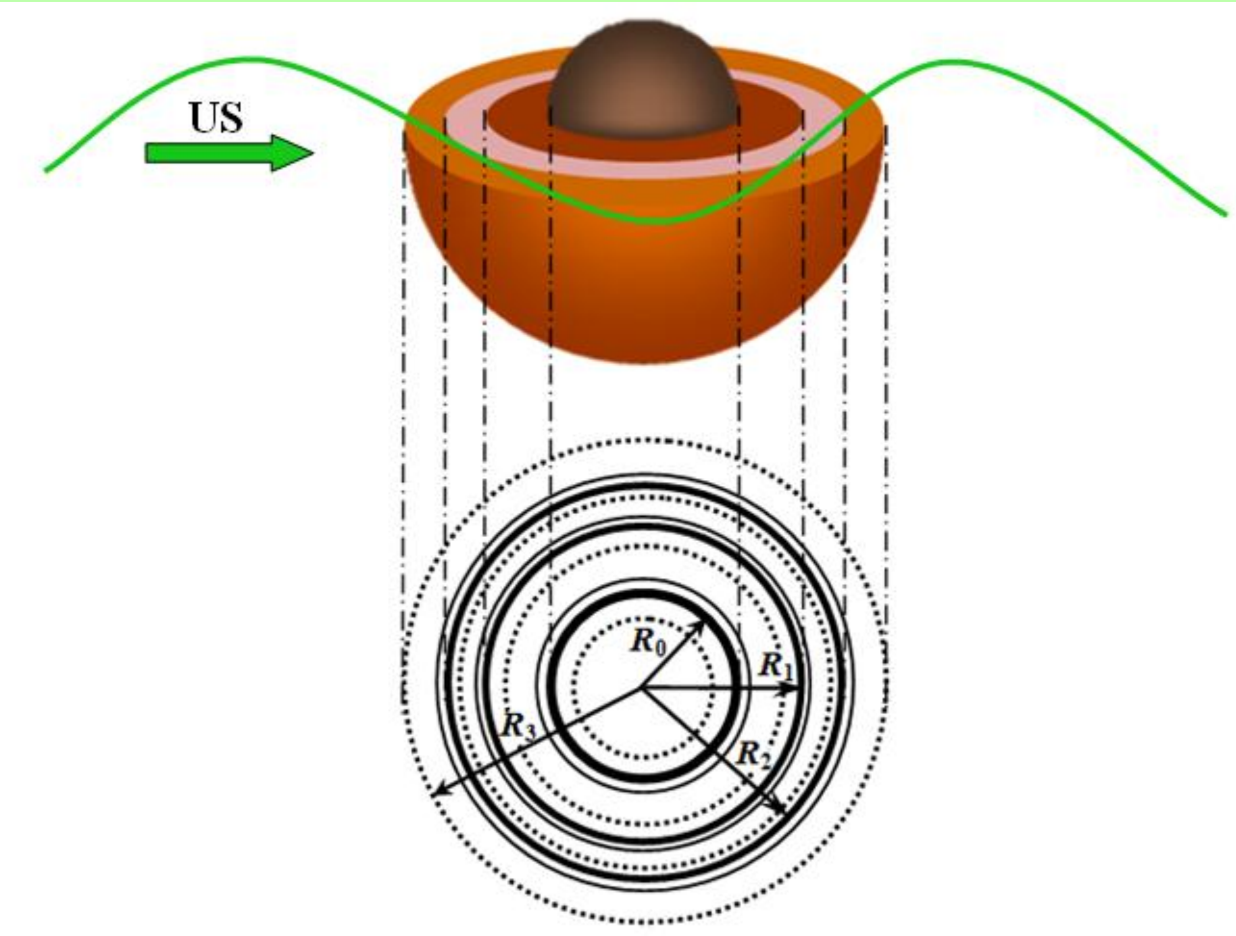

Fig. 1. The geometric model of QD of the type of CdSe-core / ZnS/CdS/ZnS-shell

THE MODEL

The shifts of the edges of both allowed energy bands as a result of elastic straining can be expressed as

$$\Delta E_c^{(i)}(t) = a_c^{(i)}\varepsilon^{(i)}(t) = \Delta E_{c1}^{(i)} + \Delta E_{c2}^{(i)}(t);$$

$$\Delta E_\upsilon^{(i)}(t) = a_\upsilon^{(i)}\varepsilon^{(i)}(t) = \Delta E_{\upsilon1}^{(i)} + \Delta E_{\upsilon2}^{(i)}(t);$$

where $\Delta E_{c1}^{(i)}$ ($\Delta E_{\upsilon1}^{(i)}$) are the energy shifts of the edges of the conduction (valence) band in the QD and shell caused by a mismatch between the lattice parameters in the contacting materials; $\Delta E_{c2}^{(i)}(t)$ and $\Delta E_{\upsilon2}^{(i)}(t)$ are their counterparts emerging owing to the action of an acoustic wave; $a_c^{(i)}$ ($a_\upsilon^{(i)}$) are the constants of the hydrostatic deformation potential of the conduction (valence) bands.

To determine the components of the strain tensor, it is necessary to find the explicit form of the displacements of atoms $\vec{u}^{(i)}(t,\vec{r})$ in QD which satisfy the equation:

$$\rho^{(i)}\frac{\partial^2 u_i^{(i)}}{\partial t^2} = \sum_j \frac{\partial \sigma_{ij}^{(i)}}{\partial x_j}, \qquad (1)$$

where $\rho^{(i)}$, $\sigma_{ij}^{(i)}$ are the density and the stress tensor

$$\sigma_{ij}^{(i)} = K^{(i)}\sum_k \varepsilon_{kk}^{(i)}\delta_{ij} + 2\mu^{(i)}\left(\varepsilon_{ij}^{(i)} - \delta_{ij}\frac{1}{3}\sum_k \varepsilon_{kk}^{(i)}\right), \qquad (2)$$

where $K^{(i)}$, $\mu^{(i)}$ are the modulus of uniform compression and the shear modulus, $\varepsilon_{ij}^{(i)}$ are the strain tensor components:

$$\varepsilon_{ij}^{(i)} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right). \qquad (3)$$

We seek the displacement vector $\vec{u}^{(i)}(t,\vec{r})$ as a sum of two terms, $\vec{u}^{(i)}(t,\vec{r}) = \vec{u}_l^{(i)}(t,\vec{r}) + \vec{u}_T^{(i)}(t,\vec{r})$, the latter satisfying the conditions:

$$\mathrm{rot}\,\vec{u}_l^{(i)}(t,\vec{r}) = 0, \quad \mathrm{div}\,\vec{u}_T^{(i)}(t,\vec{r}) = 0.$$

As a result, we obtain:

$$\Delta\vec{u}_l^{(i)} = \frac{1}{c_l^{(i)2}}\frac{\partial^2 \vec{u}_l^{(i)}}{\partial t^2}, \quad \Delta\vec{u}_T^{(i)} = \frac{1}{c_T^{(i)2}}\frac{\partial^2 \vec{u}_T^{(i)}}{\partial t^2}, \qquad (4)$$

where $c_l^{(i)} = \sqrt{\frac{3K^{(i)} + 4\mu^{(i)}}{3\rho^{(i)}}}$, $c_T^{(i)} = \sqrt{\frac{\mu^{(i)}}{\rho^{(i)}}}$ are the longitudinal and transverse, respectively, velocities of acoustically induced vibrations in the quantum dot or matrix substance.

RESULTS

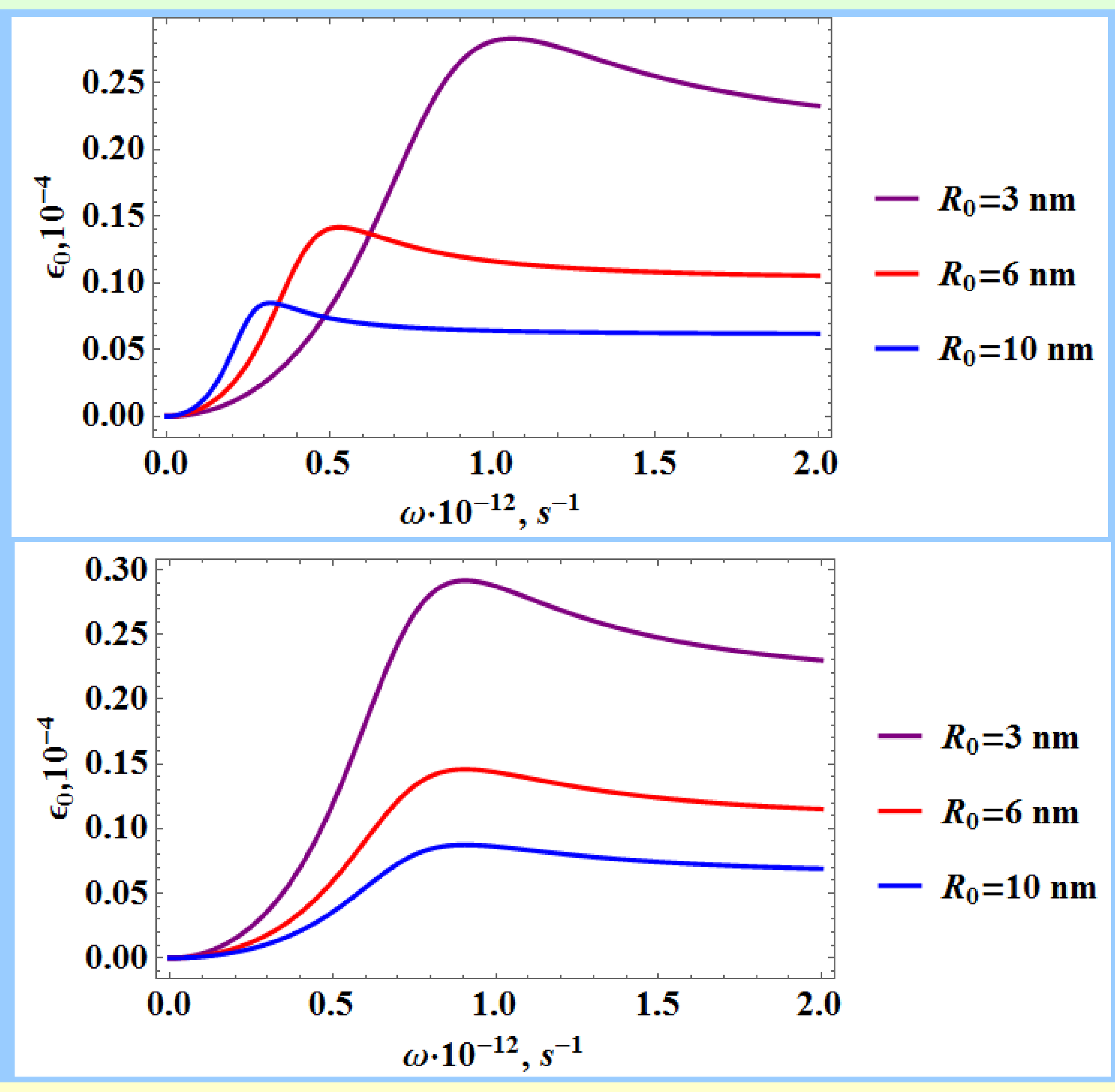

Fig 2.The dependence of the amplitude of deformation of QD material (CdSe) at the point $r=R_0$ (a) and shell material (ZnS) (b) on the frequency of the acoustic wave for different sizes of the quantum dots

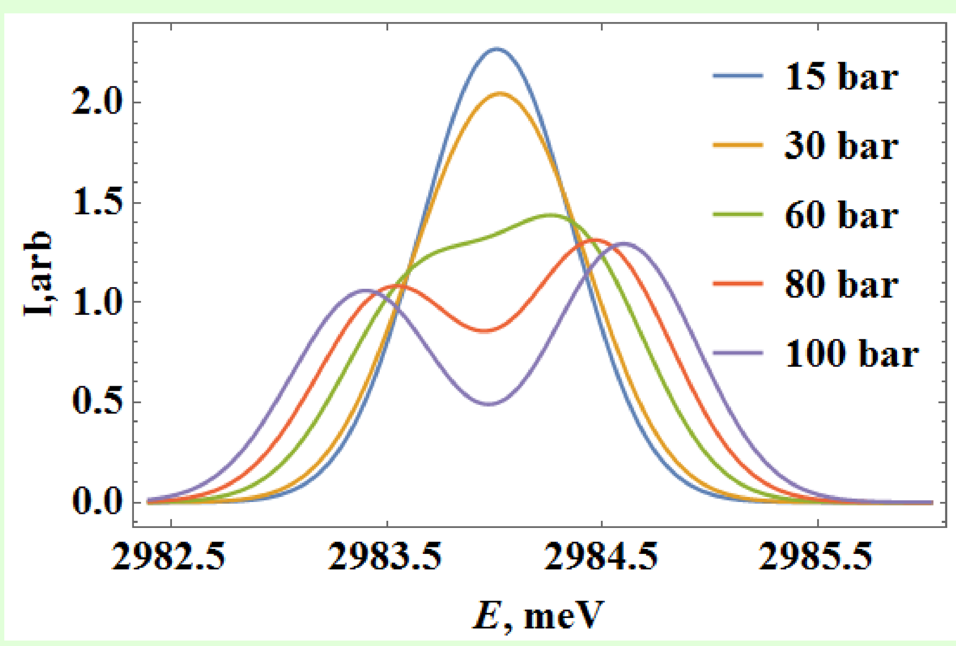

Fig. 3. The intensity of recombination radiation corresponding to the transition between the ground states of the electron and the hole in the QD of the type of CdSe-core / ZnS-shell QDs at different pressure values

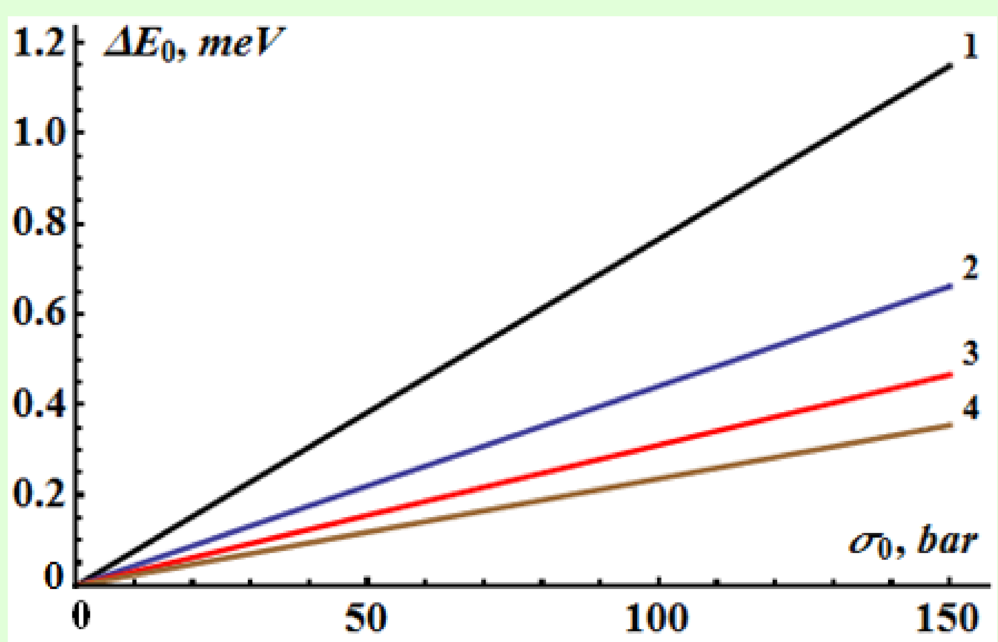

Fig. 4. The dependence of the modulation amplitude of the radiation energy that corresponds to the recombination transition between the electron and hole ground states in the CdSe/ZnS heterosystem with the CdSe QDs on the amplitude acoustic wave on the surface of the matrix: 1 - R_0 = 3 *nm*; 2 - R_0 = 5 *nm*; 3 - R_0 = 7 *nm*; 4 - R_0 = 9 *nm*

CONCLUSIONS

The electron-deformation model of nanoheterosystem with QDs, which is under influence of acoustic wave, is constructed. The uniform deformation of CdSe-core / ZnS/CdS/ZnS-shell QDs is calculated. The offered approach takes into account as a strain, caused by a misfit of parameters of lattices of contacting materials, and the influence of acoustic wave on intense state of heterosystem with QDs. Within this model it is investigated the influence of the acoustic wave on the ground state energy of electron and hole, the band gap energy and energy of recombination radiation of CdSe/ ZnS heterostructure with CdSe spherical quantum dots. The regularities of the change in the amplitude of the modulation of the energy of the recombination radiation, which corresponds to the transition between the ground states of electron and hole in the I CdSe/ ZnS heterostructure with InAs QDs, from the amplitude of the mechanical stress created by the acoustic wave on the matrix surface at different QDs sizes are established. The reduction of the QD radius is shown to result in an increase in the modulation amplitude of the radiation energy, which is explained by the growth of deformations in the QD material.

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