Baric properties of quantum dots of the type of core (CdSe) – multilayer shell (ZnS/CdS/ZnS)

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TOPICALITY and AIMS. The QDs are sensitive to deformation, so they are used as sensors of mechanical stress, to study and control the physical characteristics of nanomaterials. The influence of pressure on the physical properties of QD is also related to surface conditions (type of shell, its thickness and number of layers). Additional pressure can be created by adsorbed atoms on the surface of the QD (for example, when interacting with drugs), impurities that alloy the QD, or an acoustic wave. In this work, we construct the model of spherical QD of the type of core (CdSe) – multilayer shell (ZnS/CdS/ZnS), which undergoes comprehensive pressure, taking into account the mismatch of the lattice parameters of the contacting layers and the pressure due to the curvature of the surface.

THE MODEL

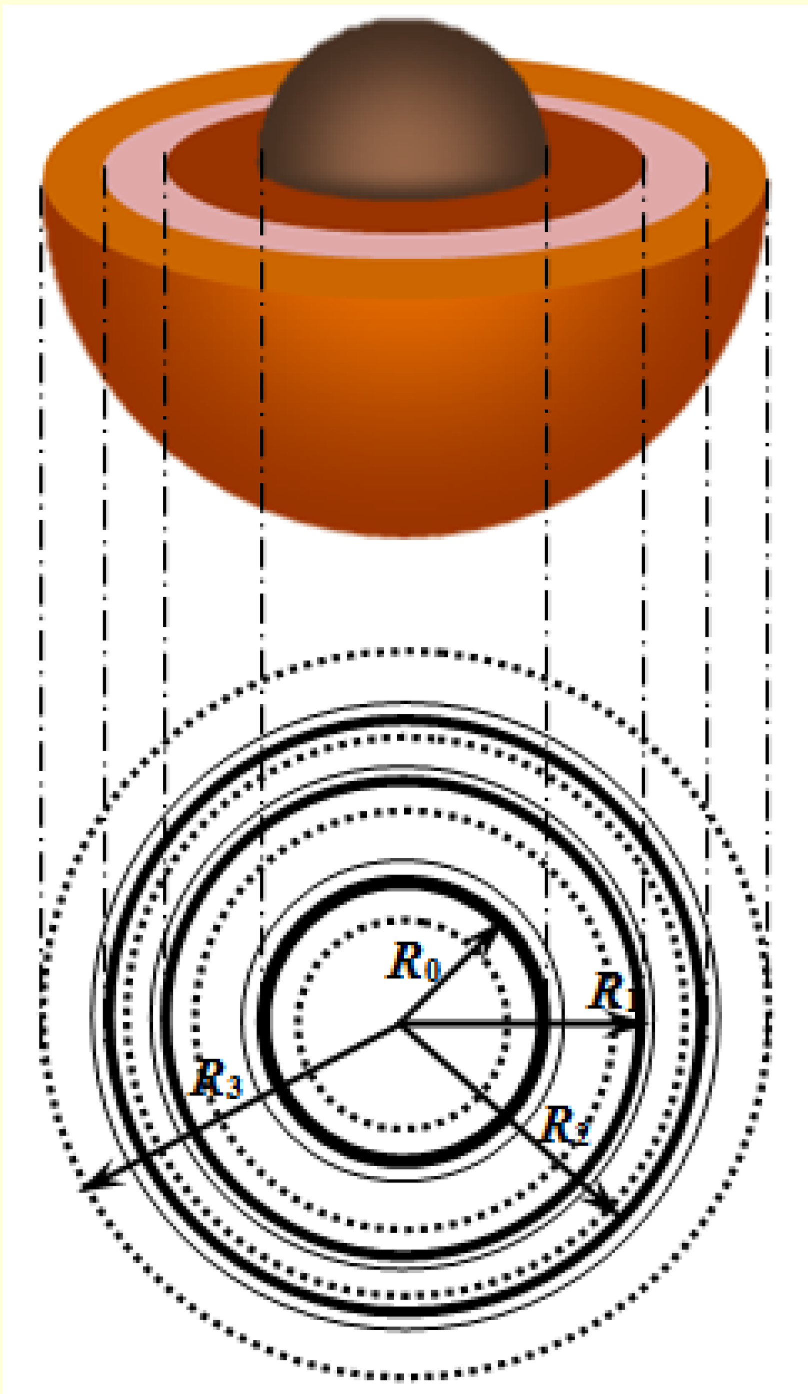

Fig. 1. The geometric model of QD of the type of CdSe-core / ZnS/CdS/ZnS-shell

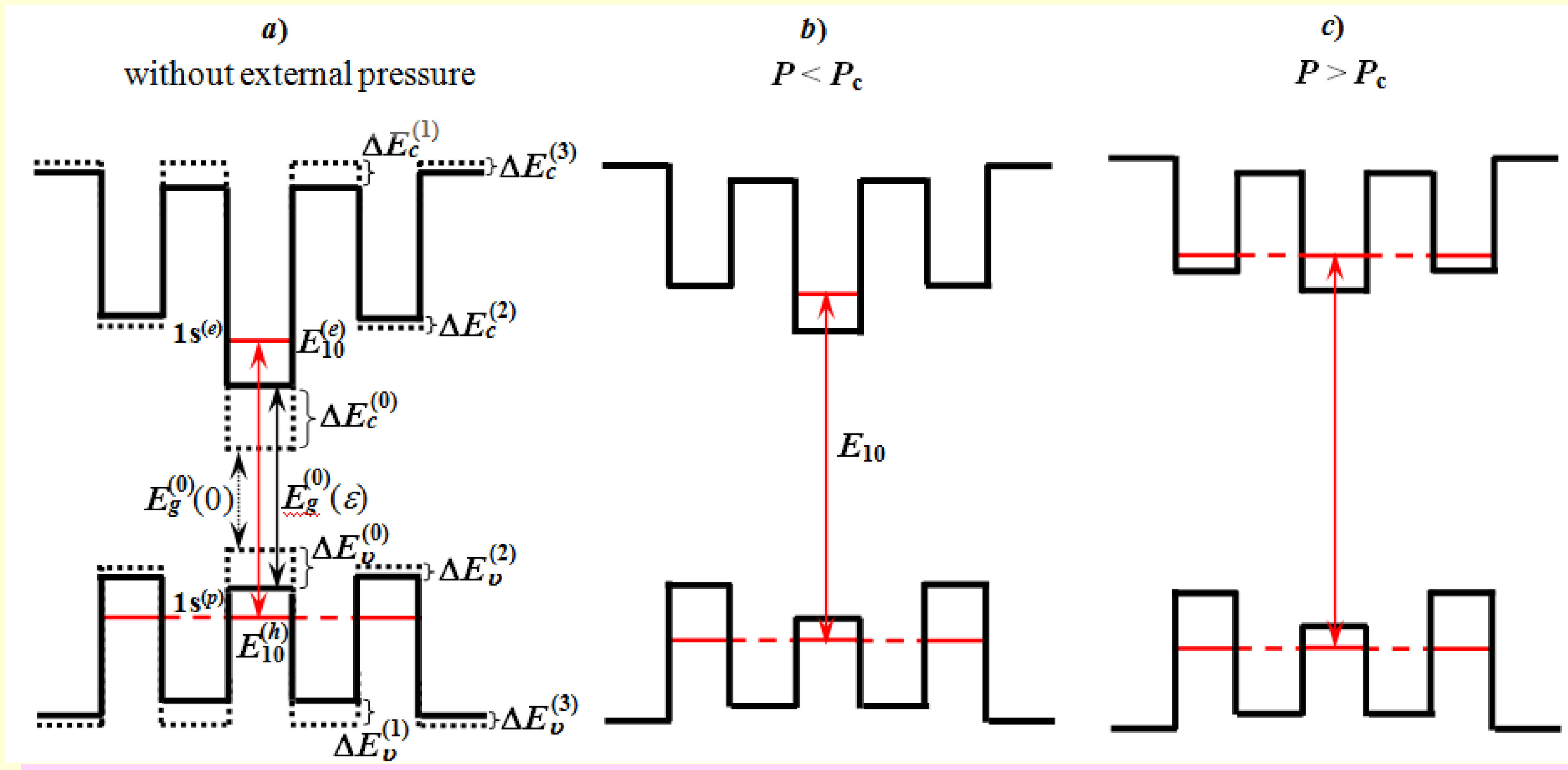

Fig. 2. The zone scheme of QD of the type of CdSe-core / ZnS/CdS/ZnS-shell (solid line) and the zone structure of the corresponding bulk materials (dotted line) in the absence of external pressure (a) and under the action of pressure (b, c)

External pressure leads to shift the edges of the allowed bands, thereby changing the energy spectrum of electrons and holes and the width of the band gap. The energy displacements of the edges of the permitted bands under the influence of elastic deformations:

$$\Delta E_c^{(i)} = a_c^{(i)}\varepsilon^{(i)}, \qquad \Delta E_\upsilon^{(i)} = a_\upsilon^{(i)}\varepsilon^{(i)}, \qquad (1)$$

where $a_c^{(i)}$, $a_\upsilon^{(i)}$ are the constants of hydrostatic deformation potential of the conduction band and valence band,

$$\varepsilon^{(i)} = \varepsilon_{rr}^{(i)} + \varepsilon_{\theta\theta}^{(i)} + \varepsilon_{\varphi\varphi}^{(i)}, \qquad i = 0 \equiv \text{CdSe}, \quad 1 \equiv \text{ZnS}, \quad 2 \equiv \text{CdS}, \quad 3 \equiv \text{ZnS}$$

To determine the components of the deformation tensor, it is necessary to find the displacements of atoms in the materials of the QD core (i = 0) and layers of shell (i = 1, 2, …, n). To do this, we will write down the equation of equilibrium (2) with the following boundary conditions (3):

$$\vec{\nabla}\operatorname{div}\vec{u} = 0 \quad (2)$$

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

where $P_L^{(i)}(R^i) = \dfrac{2\gamma^{(i)}}{R^i}$ is Laplace pressure.

The change in volume in the vicinity of the corresponding heteroboundaries is determined by the formula

$$\Delta V^{(i)} = f^{(i)} \cdot 4\pi\left(R_i^3 - R_{i-1}^3\right),$$

where $f^{(i)}$ expresses the mismatch of lattice parameters of contacting materials.

RESULTS

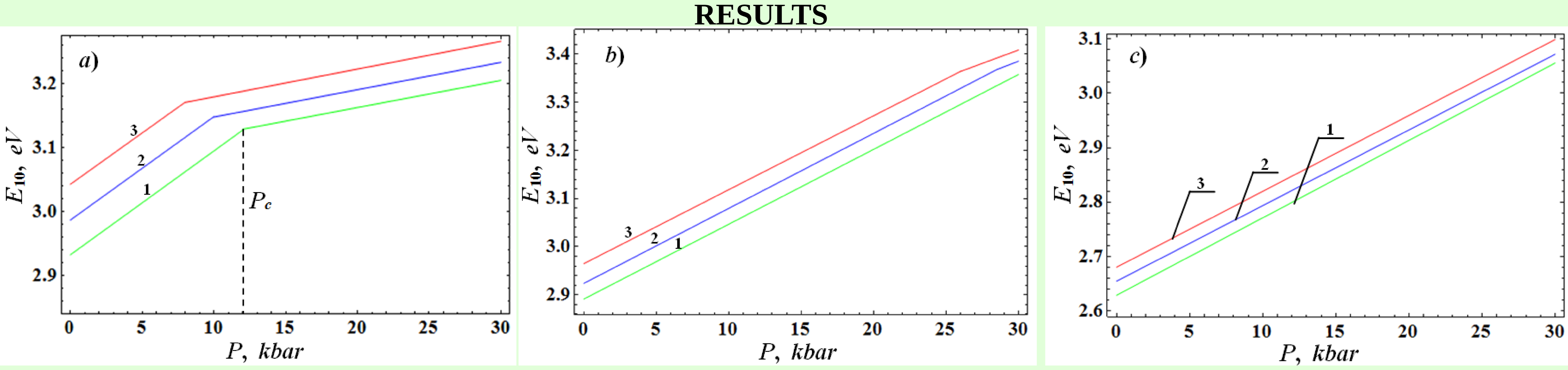

Fig. 3. The dependence of the width of the optical slit on the value of the external pressure in the QD of the type of CdSe / ZnS/CdS/ZnS at different values of the radius of the QD core (R_0 = 2 *nm* (a); R_0 = 2,4 *nm* (b); R_0 = 4 *nm* (c)) and thickness of the shell layers ($d_2 = a^{(2)}$ (1); $d_2 = 2\,a^{(2)}$ (2); $d_2 = 4\,a^{(2)}$ (3)); $d_i = R_i - R_{i-1}$ is the thickness of the i-th layer of the shell; $a^{(i)}$ is the lattice constant

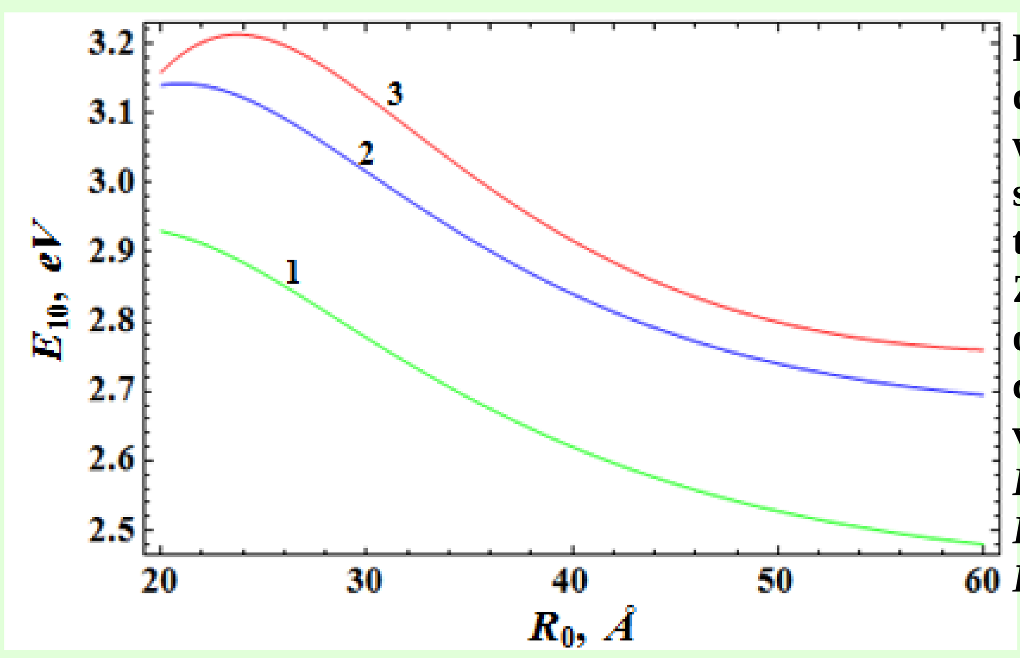

Fig. 4. The dependence of the width of the optical slit in the QD of the type of CdSe-core / ZnS/CdS/ZnS-shell on the radius of the core at different values of pressure:
***P* = 0 (1);**
***P* = 15 *kbar* (2);**
***P* = 20 *kbar* (3)**

CONCLUSIONS

The influence of external pressure on the energy structure of QD of the type of CdSe-core / ZnS/CdS/ZnS-shell is investigated within the method of deformation potential. It is shown that by changing the thickness of the shells and the value of pressure, it is possible to change the width of the optical slit of the QD in a wide range. It is established that in the case of small QD cores (less than 2,5 *nm*), depending on the value of the external pressure, two intervals of change in the width of the optical slit can be realized: at low pressures there will be a fast increase in the width of the optical slit ((15,4 -15,6) *meV/kbar*) and a slow increase at pressures greater than the critical value. This effect is explained by the fact that in the absence of pressure or at low pressures, the spherical quantum well of the CdSe core is deeper than the quantum well in the CdS layer, and, accordingly, the electron is localized in the CdSe core. The increase in pressure leads to an upward shift of the bottom of the conduction band of the material of the QD core and, accordingly, the electron may be in the material of CdSe or CdS. Since the pressure changes the deformation of CdS very little, a further increase in pressure changes very little the position of the level of an electron in the ground state. It is known that only systems with uniform in size and shape of QDs have unique properties. This is due to the fact that even a small difference in size leads to a blurring of the energy spectrum. Within the framework of the conducted researches it is established that at a certain value of pressure it is possible to provide the same width of the optical slit for QDs with different radii of cores.