Analytical approach for strain field in core multi-shell quantum dots

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The strain field in semiconductor core multi-shell quantum dots is obtained within linear continuum elasticity approach. Concrete expressions are provided for one and two shells in spherical and cylindrical symmetry. The model is applied to several typical heterostructures. The hydrostatic strain of the core is found to be strongly dependent on the thickness and elastic parameters of the shells.

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1. Introduction

As a result of their quantized electronic states, the quantum dots (QDs) have opened the way for a variety of novel device applications and meanwhile have enabled advances in fundamental physics studies of three-dimensional confined structures at the nanometer scale. Semiconductor heterostructures QDs have a wide range of applications in, for example, optoelectronic and spintronic devices, creating a demand for the development of fast and reliable methods for modeling their physical properties. The electronic structure of interfaces between lattice-mismatched semiconductors is sensitive to the strain [1,2]. One of the leading methods for growing semiconductor QDs is the molecular-beam epitaxy, by which self-assembled small islands are obtained on a thin film that is strained with respect to a substrate [3-5]. The coarsening/roughening process by which the islands are formed is a result of lattice-mismatch-induced strain. In the last decade, given the large perspective of applications in medicine, a much less expensive technique of obtaining QDs by chemical synthesis attracted the interest of scientists (see, for example, Ref. [6], and references therein). The interpretation of the electronic structure of such QDs is profoundly affected by their strain profile.

Beyond the importance in the growth mechanism itself, the strain has a crucial role in engineering the physical properties of the nanostructures. Thus, knowledge of the strain field derived from the lattices mismatch is very important since it substantially modifies the electronic band structure of semiconductor nanostructures, which, in turn, strongly affects the transport properties [7] or the performance of optoelectronic devices [8,9]. The optical spectra of semiconductor QDs are strongly influenced by strain. Thus, for an accurate simulation of the (multi)excitonic spectra, strain should be counted for both influence on the effective masses of the carriers [10] and on the existence of optical phonons modes [11,12]. The spintronics opened the way to a new class of storage and computing electronic devices. In such devices, strain is one of the control parameters. For example, in the intrinsic spin Hall effect, the conductivity of a two-dimensional electronic gas is influenced by both magnetic and strain fields [13,14] and the existence of enormous strain fields in self-assembled quantum dots has led to the expectation of dramatic effects of piezoelectricity [15-17].

Within the *continuum elasticity model* (CM), the strain distribution for isotropic or anisotropic materials is obtained by either (i) solving the elasticity equilibrium equation [16, 18], or (ii) by minimizing the elastic energy stored in the nanostructure [1,19]. In this work, given the growing interest in the core-shell (CS) QDs nanostructures, we present a theoretical CM approach for strain computation in such structures. The strain distribution is obtained by solving the linear elasticity equilibrium equation. As our modeling is developed for high symmetry structures, based on Ref.[18], where the strain for spherical QDs is practically the same for both isotropic and anisotropic treatments, we consider an isotropic treatment. The novelty character of the present work is the treatment of the strain field for multi-shell structures. Thus, differently to the treatments from the literature, which consider QD embedded in infinite matrix [1,4,16,18,19] or approximate treatments for QD with one finite shell [20,21] our model can be generalized to any number of shells. However, for practical reasons, we consider a two-shell problem. We obtain explicit analytical expressions of the strain for spherical and cylindrical symmetry, the results being very useful in the calculus of energy structures of CS nanostructures of disc, cylinder, and sphere shape, when the strain is appropriate to be taken into account within a CM approach.

The paper is structured as follows. In section 2 we present the theory used in describing the strain field. In section 3 we apply the theory to several core two-shell structures. Section 4 contains the conclusions.

2. Theory

In what follows, we consider isotropic materials described by the continuum model approach in the linear limit, in which the equilibrium equation [22], $2(1-\nu)\,\mathrm{grad}\,\mathrm{div}\,\mathbf{u}-(1-2\nu)\,\mathrm{curl}\,\mathrm{curl}\,\mathbf{u}=0$, is valid ($\nu$ is the Poisson ratio and $\mathbf{u}$ the elastic displacement field). For spherical CS structures (see Fig. 1), the lattice mismatch induces internal displacements in the radial direction *r*. On the other hand, for cylindrical symmetrical CS structures (see Fig. 1), the lattice mismatch induces internal displacements in both radial and longitudinal direction *z*. If the cylinder bases are fixed the longitudinal displacements are zero and the strain field is identical with that of a disc. For such longitudinal and/or radial displacements the field is irrotational, consequently the displacement fields are described by equation

$$\mathrm{grad}\,\mathrm{div}\,\mathbf{u}=0. \tag{1}$$

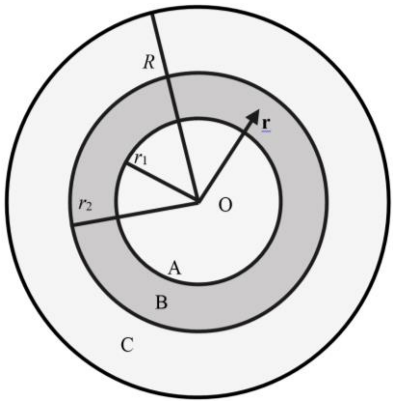

Fig. 1. Cross-section of the symmetrical spherical or cylindrical CS structure.

To find the strain tensor we adopt the following strategy. We take solutions of Eq. (1) having the form in accordance with the symmetry of the problem. Next, we compute the strain tensor components and find the stress tensor σ_{ij} by applying Hooke's law [22], $\sigma_{ij}=E(1+\nu)^{-1}\left[e_{ij}+\nu(1-2\nu)^{-1}e_{ll}\delta_{ij}\right]$ (where E is the Young modulus). Then, we require the following boundary conditions:

$$\sigma_{rr}^{A}(r_1)=\sigma_{rr}^{B}(r_1), \tag{2.1}$$

$$\sigma_{rr}^{B}(r_2)=\sigma_{rr}^{C}(r_2), \tag{2.2}$$

$$\sigma_{rr}^{C}(R)=0, \tag{2.3}$$

$$u_r^{A}(r_1)-u_r^{B}(r_1)=\varepsilon_1 r_1, \tag{2.4}$$

$$u_r^{B}(r_2)-u_r^{C}(r_2)=\varepsilon_2 r_2. \tag{2.5}$$

where $\varepsilon_1=(a_{\mathrm{B}}-a_{\mathrm{A}})/a_{\mathrm{A}}$ and $\varepsilon_2=(a_{\mathrm{C}}-a_{\mathrm{B}})/a_{\mathrm{B}}$ are the relative lattice mismatches. Eqs. (2.1-2) express the mechanical equilibrium of the interfaces, Eq. (2.3) holds for zero (negligible) pressure outside the structure, and Eqs. (2.4-5) hold for the *shrink-fit* induced by the lattice mismatch (it makes connection between a continuum approach and the crystalline structure of the materials). The strain is obtained from the solution of the system of Eqs. (2). As can easily be seen the system of equations (2) allows an immediate generalization for any number of shell.

2.1 Cylindrical symmetry

Next, we find expression of the strain for CS with cylindrical symmetry for two shells and then by reduction for one shell.

a) Cylinder with fixed bases

For cylindrical CS with fixed bases or disc CS, as we already specified, the solutions are identical. The displacement written in the usual cylindrical coordinates takes the form, $\mathbf{u}=(u_r(r),0,0)$. We search for solutions of the form $u_r^{X}(r)=X_1 r+X_2/r$, with X = A (the core), B or C (the first or second shell, respectively), see Fig.1. $A_1, A_2, B_1, B_2, C_1, C_2$ are constants and we take $A_2=0$ to avoid singularity.

a.1) Two shells

Following the above procedure, we obtain the strain tensor components. Their non-zero expressions in the limit of similar elastic constants, $\nu_A=\nu_B=\nu_C=\nu$, $E_A=E_B=E_C$ are as follows:

$$e_{rr}^{\mathrm{A}}=e_{\theta\theta}^{\mathrm{A}}=\frac{1}{2}\frac{1-2\nu}{1-\nu}\left[\varepsilon_1\left(1-\frac{r_1^2}{R^2}\right)+\varepsilon_2\left(1-\frac{r_2^2}{R^2}\right)\right] \tag{3.1}$$

$$e_{hyd}^{\mathrm{A}}=\frac{1-2\nu}{1-\nu}\left[\varepsilon_1\left(1-\frac{r_1^2}{R^2}\right)+\varepsilon_2\left(1-\frac{r_2^2}{R^2}\right)\right] \tag{3.2}$$

$$e_{\substack{rr,\\ \theta\theta}}^{\mathrm{B}}(r)=\frac{1-2\nu}{1-\nu}\left[-\varepsilon_1\frac{r_1^2}{R^2}\left(1\mp\frac{1}{1-2\nu}\frac{R^2}{r^2}\right)+\varepsilon_2\left(1-\frac{r_2^2}{R^2}\right)\right] \tag{3.3}$$

$$e_{hyd}^{\mathrm{B}}=\frac{1-2\nu}{1-\nu}\left[-\varepsilon_1\frac{r_1^2}{R^2}+\varepsilon_2\left(1-\frac{r_2^2}{R^2}\right)\right] \tag{3.4}$$

$$e_{\substack{rr\\ \theta\theta}}^{\mathrm{C}}(r)=-\frac{1}{2}\frac{1-2\nu}{1-\nu}\left(1\mp\frac{1}{1-2\nu}\frac{R^2}{r^2}\right)\left(\varepsilon_1\frac{r_1^2}{R^2}+\varepsilon_2\frac{r_2^2}{R^2}\right) \tag{3.5}$$

$$e_{hyd}^{\mathrm{C}}=-\frac{1-2\nu}{1-\nu}\left(\varepsilon_1\frac{r_1^2}{R^2}+\varepsilon_2\frac{r_2^2}{R^2}\right) \tag{3.6}$$

In Appendix, we give the complete expressions.

a.2) One shell

By taking $r_1=r_0$, $r_2=R$, and $\varepsilon_1=\varepsilon_0$, we collapse the two shells and reduce the problem to that of only one shell. The non-zero expressions of the strain tensor components

in the limit of similar elastic constants, $\nu_A = \nu_B = \nu$, $E_A = E_B$ are as follows:

$$e_{rr}^{\mathrm{A}} = e_{\theta\theta}^{\mathrm{A}} = \varepsilon_0 \frac{1}{2}\frac{1-2\nu}{1-\nu}\left(1-\frac{r_0^2}{R^2}\right) \to \varepsilon_0 \frac{1}{2}\frac{1-2\nu}{1-\nu}, \quad (4.1)$$

$$e_{hyd}^{\mathrm{A}} = \varepsilon_0 \frac{1-2\nu}{1-\nu}\left(1-\frac{r_0^2}{R^2}\right) \to \varepsilon_0 \frac{1-2\nu}{1-\nu}, \quad (4.2)$$

$$e_{\substack{rr,\\ \theta\theta}}^{\mathrm{B}}(r) = \varepsilon_0 \frac{1}{2}\frac{1}{1-\nu}\left(\pm\frac{r_0^2}{r^2} - (1-2\nu)\frac{r_0^2}{R^2}\right) \to \pm\varepsilon_0 \frac{1}{2}\frac{1}{1-\nu}\frac{r_0^2}{r^2} \quad (4.3)$$

$$e_{hyd}^{\mathrm{B}} = -\varepsilon_0 \frac{(1-2\nu)}{(1-\nu)}\frac{r_0^2}{R^2} \to 0. \quad (4.4)$$

(where $\to$ stands for $R \to \infty$).

We observe the calculus correctness and the physical tests are checked since e_{rr}^{A}, $e_{\theta\theta}^{\mathrm{A}}$, e_{hyd}^{A} vanish when $r_0 = R$ (no shell and no pressure outside the core), e_{hyd}^{B} vanishes for thick shell, and $e_{rr}^{\mathrm{B}}(r)$, $e_{\theta\theta}^{\mathrm{B}}(r)$ vanish for large R at large distance of the QD center. In Appendix, we give the complete expressions.

b) Cylinder with free bases and one shell

For cylindrical CS with *free* bases, the displacement takes the form $\mathbf{u} = (u_r(r), 0, u_z(z))$ and modeling the longitudinal strain makes the algebra more complex. Next, we consider a usual simplification [4] and take $e_{zz}^{A}(z) = \varepsilon_0$ and $e_{zz}^{B}(z) = 0$, which holds for thick shell (in longitudinal direction the lattice constant of the core becomes that of the shell and the lattice constant of the shell does not change). By repeating the procedure we described, we obtain:

$$e_{rr}^{\mathrm{A}} = e_{\theta\theta}^{\mathrm{A}} = \varepsilon_0 \frac{1}{2}\frac{1-3\nu+(1+\nu)(1-2\nu)r_0^2/R^2}{1-\nu} \to \varepsilon_0 \frac{1}{2}\frac{1-3\nu}{1-\nu} \quad (5.1)$$

$$e_{hyd}^{\mathrm{A}} = \varepsilon_0 \frac{1-2\nu}{1-\nu}\left[2-(1+\nu)r_0^2/R^2\right] \to 2\varepsilon_0 \frac{1-2\nu}{1-\nu} \quad (5.2)$$

$$e_{\substack{rr,\\ \theta\theta}}^{\mathrm{B}}(r) = -\varepsilon_0 \frac{1}{2}\frac{1+\nu}{1-\nu}\left(\mp R^2/r^2 + 1 - 2\nu\right)\frac{r_0^2}{R^2} \to \pm\varepsilon_0 \frac{1}{2}\frac{1+\nu}{1-\nu}\frac{r_0^2}{r^2} \quad (5.3)$$

$$e_{hyd}^{\mathrm{B}} = -\varepsilon_0 \frac{1+\nu}{1-\nu}(1-2\nu)\frac{r_0^2}{R^2} \to 0 \quad (5.4)$$

Thus, we recover the results of Grundmann [4] for thick shell ($R \to \infty$). In Appendix, we give the complete expressions.

2.2 Spherical symmetry

Next, we find expression of the strain for CS with spherical symmetry for two shells and then by reduction for one shell. The displacement written in the usual spherical coordinates takes the form $\mathbf{u} = (u_r(r), 0, 0)$.

1) Two shells

We search for solutions of the form $u_r^X(r) = X_1 r + X_2/r^2$, with the same meaning of X as in the cylinder case. Following the same procedure, we find the strain tensor components. Their non-zero expressions in the limit of similar elastic constants, $\nu_A = \nu_B = \nu_C = \nu$, $E_A = E_B = E_C$ are as follows:

$$e_{rr}^{A} = e_{\theta\theta}^{A} = e_{\varphi\varphi}^{A} = \frac{2}{3}\frac{1-2\nu}{1-\nu}\left[\varepsilon_1\left(1-r_1^3/R^3\right) + \varepsilon_2\left(1-r_2^3/R^3\right)\right] \quad (6.1)$$

$$e_{hyd}^{A} = 2\frac{1-2\nu}{1-\nu}\left[\varepsilon_1\left(1-r_1^3/R^3\right) + \varepsilon_2\left(1-r_2^3/R^3\right)\right], \quad (6.2)$$

$$e_{rr}^{B}(r) = \frac{2}{3}\frac{1-2\nu}{1-\nu}\left(\varepsilon_1\frac{r_1^3}{R^3}\left(\frac{R^3}{r^3}\frac{1+\nu}{1-2\nu}-1\right) + \varepsilon_2\left(1-\frac{r_2^3}{R^3}\right)\right), \quad (6.3)$$

$$e_{\theta\theta}^{B}(r) = e_{\varphi\varphi}^{B}(r) = \frac{2}{3}\frac{1-2\nu}{1-\nu}\left(-\varepsilon_1\frac{r_1^3}{R^3}\left(\frac{1}{2}\frac{R^3}{r^3}\frac{1+\nu}{1-2\nu}+1\right) + \varepsilon_2\left(1-\frac{r_2^3}{R^3}\right)\right) \quad (6.4)$$

$$e_{hyd}^{B} = 2\frac{1-2\nu}{1-\nu}\left(-\varepsilon_1\frac{r_1^3}{R^3} + \varepsilon_2\left(1-\frac{r_2^3}{R^3}\right)\right), \quad (6.5)$$

$$e_{rr}^{C}(r) = \frac{2}{3}\frac{1-2\nu}{1-\nu}\left(\frac{R^3}{r^3}\frac{1+\nu}{1-2\nu}-1\right)\left(\varepsilon_1\frac{r_1^3}{R^3} + \varepsilon_2\frac{r_2^3}{R^3}\right), \quad (6.6)$$

$$e_{\theta\theta}^{C}(r) = e_{\varphi\varphi}^{C}(r) = -\frac{2}{3}\frac{1-2\nu}{1-\nu}\left(\frac{1}{2}\frac{R^3}{r^3}\frac{1+\nu}{1-2\nu}+1\right)\left(\varepsilon_1\frac{r_1^3}{R^3} + \varepsilon_2\frac{r_2^3}{R^3}\right) \quad (6.7)$$

$$e_{hyd}^{C} = -2\frac{1-2\nu}{1-\nu}\left(\varepsilon_1\frac{r_1^3}{R^3} + \varepsilon_2\frac{r_2^3}{R^3}\right) \quad (6.8)$$

2) One shell

By taking $r_1 = r_0$, $r_2 = R$, and $\varepsilon_1 = \varepsilon_0$, we collapse the two shells and reduce the problem to that of only one shell. The non-zero expressions of the strain tensor components in the limit of similar elastic constants, $\nu_A = \nu_B = \nu$, $E_A = E_B$ are as follows:

$$e_{rr}^{A} = e_{\theta\theta}^{A} = e_{\varphi\varphi}^{A} = \varepsilon_0 \frac{2}{3}\frac{1-2\nu}{1-\nu}\left(1-\frac{r_0^3}{R^3}\right) \to \varepsilon_0 \frac{2}{3}\frac{1-2\nu}{1-\nu} \quad (7.1)$$

$$e_{hyd}^{A} = 2\varepsilon_0 \frac{1-2\nu}{1-\nu}\left(1-\frac{r_0^3}{R^3}\right) \to 2\varepsilon_0 \frac{1-2\nu}{1-\nu} \quad (7.2)$$

$$e_{rr}^{B}(r) = \varepsilon_0 \frac{2}{3}\frac{1-2\nu}{1-\nu}\frac{r_0^3}{R^3}\left(\frac{R^3}{r^3}\frac{1+\nu}{1-2\nu}-1\right) \to \varepsilon_0 \frac{2}{3}\frac{1+\nu}{1-\nu}\frac{r_0^3}{r^3} \quad (7.3)$$

$$e_{\theta\theta}^{B}(r) = e_{\varphi\varphi}^{B}(r) = -\varepsilon_0 \frac{2}{3}\frac{1-2\nu}{1-\nu}\frac{r_0^3}{R^3}\left(\frac{1}{2}\frac{R^3}{r^3}\frac{1+\nu}{1-2\nu}+1\right) \to -\varepsilon_0 \frac{1}{3}\frac{1+\nu}{1-\nu}\frac{r_0^3}{r^3} \quad (7.4)$$

$$e_{hyd}^{B} = -2\,\varepsilon_0 \frac{1-2\nu}{1-\nu}\frac{r_0^3}{R^3} \to 0 \qquad (7.5)$$

We notice that eqs (7.1-5) provide the same expressions for the tensor components in a CS QD as in Ref.[21] and in the limit $R \to \infty$ we get the same results as in Ref.[4].

3. Applications. Results

Even in the most symmetric crystalline structure, the cubic system, the Young modulus and Poisson ratio vary with direction. On the other hand, as we already specified, the isotropic treatment we consider is justified for highly symmetry structures [18] (the influence of the elastic anisotropy is very small for sphere). In this isotropic limit, the elastic parameters are obtained by identifying the linear relation between stress and strain written with the stiffness tensor [23] for the (cubic here) crystal with Hooke's law. One immediately finds:

$$E = \frac{C_{11}^2 + C_{11}C_{12} - 2C_{12}^2}{C_{11} + C_{12}} \text{ and } \nu = \frac{C_{12}}{C_{11} + C_{12}}\,.$$

3.1 Disc shape QDs

As a first example, we consider an in-plane disc graphene QD. We show the strain distribution for a QD with a honeycomb graphene lattice core (r_0=2nm) which is coated with a hydrogenated form of graphene, the isotropic C-graphane [24] (shell thickness of 0.4nm). For the elastic parameters, we consider the values obtained using the elastic constants C_{11} and C_{12} in Ref. [24]. Thus, ν_{graphene}=0.145, E_{graphene}=3.37·10^{11} Nm^{-2}, ν_{graphane}=0.075 and E_{graphane}=2.45·10^{11} Nm^{-2}. The lattice constants from the same Ref. [24], a_{graphene}=2.46Å, a_{graphane}=2.54Å, give a positive ε = 3.25%. In Fig. 2 one shows the expected behavior, the graphene core is stretched ($e_{hyd}^{graphene} > 0$) and the C-graphane shell is compressed ($e_{hyd}^{graphane} < 0$). The high value of the hydrostatic strain obtained for the graphene/C-graphane QD indicates that a simulation of the energy structure of such a nanostructure should consider the strain in computation as one of the major importance ingredient in the study.

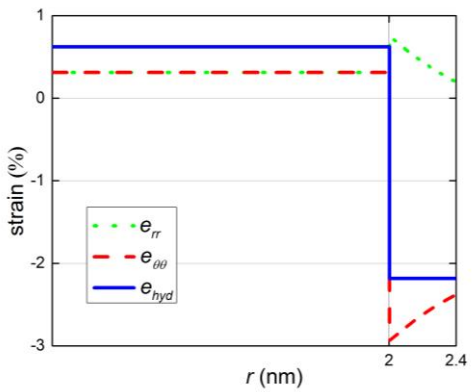

Fig. 2. Strain distribution in a graphene/C-graphane QD.

3.2 Spherical QD

As Eqs. (A1) or (B1) show, the strain of each material is dependent on two factors: (i) the elastic parameters (E and ν) and (ii) the relative lattice mismatches (ε). Modifying these two factors various strain field distributions can be obtained. It is interesting to investigate the case in which, by adjusting the properties of the second shell (or by finding an appropriate material), the elastic state of the core can be reversed from compressed to stretched or vice versa.

To illustrate the phenomenon, we consider ZnS/CdS/ZnS QD [25] with radii r_1 = 1.8 nm, r_2 = 2.4 nm, R = 3.2 nm. The lattice constant for ZnS (a_{ZnS}=5.40Å [26]) is considerably smaller ($\varepsilon_1 \approx$ 7.5%) than for CdS (a_{CdS}=5.82Å [27]); the relative lattice mismatch between the CdS and the second shell of ZnS is negative ($\varepsilon_2 \approx$ -7.5%). Here only, we redefined the relative lattice mismatch as ε=(a_{out}-a_{in})/a_{average} with a_{average}=(a_{out}+a_{in})/2.

The parameters E and ν are calculated for ZnS with the elastic constants from Ref. [26]: ν_{ZnS} = 0.384, E_{ZnS} = 5.55·10^{10} Nm^{-2} and for CdS with those from Ref. [28]: ν_{CdS} = 0.406 and E_{CdS} = 2.99·10^{10} Nm^{-2}. We obtain the core is expanded, $e_{hyd}^{A} > 0$ (see Fig. 3) and conclude that the above factor (ii) has a stronger impact. As expected, the second shell is expanded, too. If we hypothetically increase the Young modulus of the second shell (by 60% here) the factor (i) becomes more significant: we obtain a compressed core, $e_{hyd}^{A} < 0$ (see Fig. 4), but the second shell is still expanded. In practice, this behavior can be obtained if we replace the second shell with a suitable material, with a lattice constant close to that of ZnS but with larger Young modulus.

As a second application for spherical CS QDs, we consider silica (SiO_2) coated CdSe/CdS QDs as described in Ref. [29]. The photoluminescence (PL) intensity of the nanostructure drops with the thickness of the coating shell, but the peak position does not change (see Fig 5.2 from Ref. [29]). Depending on the mechanical conditions of the system, the polymorph silica can have different lattice configurations. With our model we can approximate which lattice constant the coating shell has by studying the strain in the core. As the main PL peak depends on the band gap QD and, on the other hand, the band is dependent on the strain field (mainly by the hydrostatic strain), we can conclude that the shell thickness influences less e_{hyd}^{CdSe}. By analyzing the functions $e_{hyd}^{CdSe} = f(R)$ for different lattice constants for the silica coating, we should choose the R dependence of e_{hyd}^{CdSe} with the shortest abrupt decay followed by constant value. For exemplification, we consider a CdSe/CdS QD with r_1=2nm and r_2=2.3nm. We observe that the hydrostatic strain of the core changes very weakly with the thickness of the coat from approximately R=6nm.This behavior is obtained for a lattice constant a_{silica}=5.963Å (see Fig. 5).

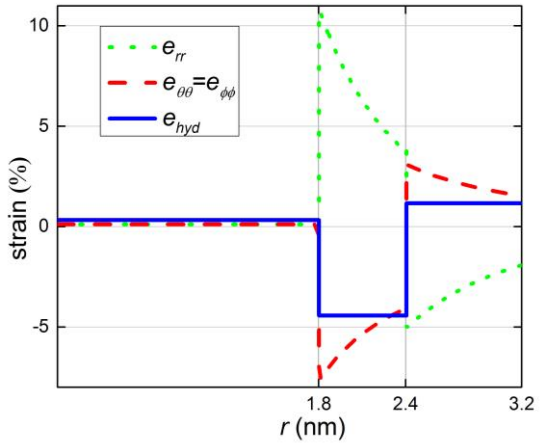

Fig. 3. Strain distribution in ZnS/CdS/ZnS QD.

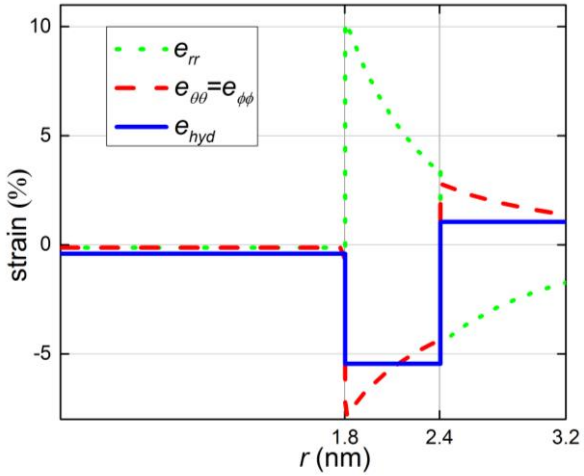

Fig. 4. Strain distribution in ZnS/CdS/modified ZnS QD.

4. Conclusions

Our isotropic CM model provides, in principle, analytical expressions of the strain field for any QD configuration with circular or spherical symmetry. The present work focuses only on the core/shell/shell system for practical reasons. Our theoretical results extend knowledge in the strain field of CS QDs and cover existent reports in the literature regarding its value [4, 20, 21, 30]. Our results on the strain field can be very useful to the energy structure simulations of CS QDs, where usually (from computational reasons) such isotropic modeling is taken into account. Interesting is the fact that though simple, the model is able to guide strain engineering in QDs by coating them with materials with certain elastic properties.

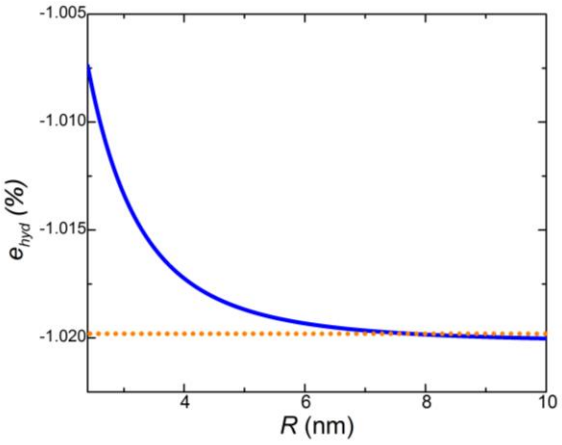

Fig. 5. The dependence of e_{hyd}^{CdSe} with the thickness of the silica shell.

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Appendix: Strain calculation

The complete expressions of the non-zero strain tensor components are as follows. In order to be easy readable, we made some notations: for example, C_3^B is the **3**rd notation made for the **C**ylinder, for B, the first shell.

A. Cylindrical symmetry

a.1) Cylindrical QD with fixed bases and two shells

$$e_{rr}^A = e_{\theta\theta}^A = \frac{\varepsilon_1 C_1^A + \varepsilon_2 C_2^A}{C_1^A + C_3^A} \tag{A1.1}$$

$$e_{hyd}^A = 2\frac{\varepsilon_1 C_1^A + \varepsilon_2 C_2^A}{C_1^A + C_3^A} \tag{A1.2}$$

where

$$C_1^A = \frac{E_B}{E_C}\frac{1+\nu_C}{1+\nu_B}\frac{r_1^2/r_2^2-1}{R^2/r_2^2-1} - \frac{1-2\nu_B+r_1^2/r_2^2}{1-2\nu_C+R^2/r_2^2}, C_2^A = \frac{-2(1-\nu_B)}{1-2\nu_C+R^2/r_2^2}$$

,

$$C_3^A = \frac{E_A}{(1-2\nu_A)(1+\nu_A)}\left(\frac{1+\nu_B}{E_B}\frac{(1-2\nu_B)\left(r_1^2/r_2^2-1\right)}{1-2\nu_C+R^2/r_2^2} - \frac{1+\nu_C}{E_C}\frac{1+(1-2\nu_B)r_1^2/r_2^2}{R^2/r_2^2-1}\right).$$

$$e_{rr\,\theta\theta}^B(r) = \frac{\varepsilon_1 C_{1^*}^B r_1^2/r_2^2 + \varepsilon_2 C_{2^*}^B}{C_3^B} \pm \frac{r_1^2}{r^2}\frac{\varepsilon_1(1+C_1^B)+\varepsilon_2(1+C_2^B)}{C_3^B}, \tag{A1.3}$$

$$e_{hyd}^B(r) = 2\frac{\varepsilon_1 C_{1^*}^B r_1^2/r_2^2 + \varepsilon_2 C_{2^*}^B}{C_3^B}, \tag{A1.4}$$

in which $C_{1^*,2^*}^B = 1 - C_{1,2}^B(1-2\nu_B)$,

$$C_1^B=\frac{E_B}{E_C}\frac{1+\nu_C}{1+\nu_B}\frac{1-2\nu_C+R^2/r_2^2}{(1-2\nu_B)\left(R^2/r_2^2-1\right)},\ C_2^B=-\frac{E_B}{E_A}\frac{1-2\nu_A}{1-2\nu_B}\frac{1+\nu_A}{1+\nu_B},$$

$$C_3^B=1-\frac{r_1^2}{r_2^2}+C_1^B\left(1+\frac{r_1^2}{r_2^2}(1-2\nu_B)\right)-C_2^B\left[\frac{r_1^2}{r_2^2}+(1-2\nu_B)\left(1-C_1^B\left(\frac{r_1^2}{r_2^2}-1\right)\right)\right].$$

$$e_{rr}^C(r)=-\frac{\varepsilon_1C_1^C+\varepsilon_2C_2^C}{C_3^C}\left(1\mp\frac{1}{1-2\nu_C}\frac{R^2}{r^2}\right),\qquad\text{(A1.5)}$$

$$e_{hyd}^C=-2\frac{\varepsilon_1C_1^C+\varepsilon_2C_2^C}{C_3^C},\qquad\text{(A1.6)}$$

where

$$C_1^C=2\frac{r_1^2}{r_2^2}\left(1-\nu_B\right),\ C_2^C=1+(1-2\nu_B)\frac{r_1^2}{r_2^2}-\frac{E_B}{E_A}\frac{1+\nu_A}{1+\nu_B}(1-2\nu_A)\left(\frac{r_1^2}{r_2^2}-1\right)$$

,

$$C_3^C=\left(R^2/r_2^2-1\right)\left[C_{4,AC}^C\left(\frac{r_1^2}{r_2^2}+1-2\nu_B\right)-C_{4,BC}^C\left(\frac{r_1^2}{r_2^2}-1\right)\right]+C_2^C\left(\frac{R^2/r_2^2}{(1-2\nu_C)}+1\right)$$

and $C_{4,AC}^C=\frac{E_C}{E_A}\frac{1-2\nu_A}{1-2\nu_C}\frac{1+\nu_A}{1+\nu_C}$, $C_{4,BC}^C=\frac{E_C}{E_B}\frac{1-2\nu_B}{1-2\nu_C}\frac{1+\nu_B}{1+\nu_C}$.

a.2) Cylindrical QD with fixed bases and one shell

$$e_{rr}^{\mathrm{A}}=e_{\theta\theta}^{\mathrm{A}}=\varepsilon_0C_1^{AB},\qquad\text{(A2.1)}$$

$$e_{hyd}^{\mathrm{A}}=2\varepsilon_0C_1^{AB},\qquad\text{(A2.2)}$$

with $C_1^{AB}=\left[1+\frac{E_A}{E_B}\frac{1+\nu_{\mathrm{B}}}{1+\nu_{\mathrm{A}}}\frac{1+(1-2\nu_{\mathrm{B}})\,r_0^2/R^2}{(1-2\nu_A)(1-r_0^2/R^2)}\right]^{-1}$.

$$e_{\substack{rr,\\ \theta\theta}}^{\mathrm{B}}(r)=-\varepsilon_0C_4^B\left[1\mp\frac{R^2}{(1-2\nu_B)r^2}\right],\qquad\text{(A2.3)}$$

$$e_{hyd}^{\mathrm{B}}=-2\varepsilon_0C_4^B,\qquad\text{(A2.4)}$$

with $C_4^B=\left[1+\frac{R^2/r_0^2}{1-2\nu_B}+\frac{E_B}{E_A}\frac{1+\nu_A}{1+\nu_B}\frac{1-2\nu_A}{1-2\nu_B}\left(R^2/r_0^2-1\right)\right]^{-1}$.

b) Cylindrical QD with free bases and one shell

$$e_{rr}^{\mathrm{A}}=e_{\theta\theta}^{\mathrm{A}}=\varepsilon_0C_1^{AB}\left(1-\nu_A\left(\frac{1}{C_1^{AB}}-1\right)\right),\qquad\text{(A3.1)}$$

$$e_{hyd}^{\mathrm{A}}=\varepsilon_0C_1^{AB}\left(3+\left(\frac{1}{C_1^{AB}}-1\right)(1-2\nu_A)\right).\qquad\text{(A3.2)}$$

$$e_{rr}^{\mathrm{B}}(r)=-\varepsilon_0C_5^B\frac{E_B}{E_A}\left(1-\frac{R^2/r^2}{1-2\nu_A}\right),\qquad\text{(A3.3)}$$

$$e_{\theta\theta}^{\mathrm{B}}(r)=-\varepsilon_0C_5^B\left(\frac{R^2/r^2}{1-2\nu_A}+1\right),\qquad\text{(A3.4)}$$

$$e_{hyd}^{\mathrm{B}}=-2\varepsilon_0C_5^B\left(1-2\nu_B\right),\qquad\text{(A3.5)}$$

where $C_5^B=C_1^{AB}\frac{E_A}{E_B}\frac{1+\nu_{\mathrm{B}}}{R^2/r_0^2-1}$ and C_1^{AB} is the same as in a.2).

B. Spherical symmetry

1) Spherical QD with two shells

$$e_{rr}^A=e_{\theta\theta}^A=e_{\varphi\varphi}^A=\frac{\varepsilon_1S_1^A+\varepsilon_2S_2^A}{S_1^A+S_3^A},\qquad\text{(B1.1)}$$

$$e_{hyd}^A=3\frac{\varepsilon_1S_1^A+\varepsilon_2S_2^A}{S_1^A+S_3^A},\qquad\text{(B1.2)}$$

where $S_1^A=\frac{E_B}{E_C}\frac{r_1^3/r_2^3-1}{R^3/r_2^3-1}-\frac{2(1-2\nu_B)+(1+\nu_B)r_1^3/r_2^3}{2(1-2\nu_C)+(1+\nu_C)R^3/r_2^3}$,

$S_2^A=-\frac{3(1-\nu_B)}{2(1-2\nu_C)+(1+\nu_C)R^3/r_2^3}$ and

$$S_3^A=\frac{E_A}{1-2\nu_A}\left(\frac{1}{E_B}\frac{(1-2\nu_B)(1+\nu_B)\left(r_1^3/r_2^3-1\right)}{2(1-2\nu_C)+(1+\nu_C)R^3/r_2^3}-\frac{1}{E_C}\frac{(1+\nu_B)/2+(1-2\nu_B)r_1^3/r_2^3}{R^3/r_2^3-1}\right)$$

$$e_{rr}^B(r)=\frac{\varepsilon_1S_{1*}^Br_1^3/r_2^3+\varepsilon_2S_{2*}^B}{S_3^B}+2\frac{r_1^3}{r^3}\frac{\varepsilon_1(1+S_1^B)+\varepsilon_2(1+S_2^B)}{S_3^B}\qquad\text{(B1.3)}$$

$$e_{\theta\theta}^B(r)=e_{\varphi\varphi}^B(r)=\frac{\varepsilon_1S_{1*}^Br_1^3/r_2^3+\varepsilon_2S_{2*}^B}{S_3^B}-\frac{r_1^3}{r^3}\frac{\varepsilon_1(1+S_1^B)+\varepsilon_2(1+S_2^B)}{S_3^B}\qquad\text{(B1.4)}$$

$$e_{hyd}^B=3\frac{\varepsilon_1S_{1*}^Br_1^3/r_2^3+\varepsilon_2S_{2*}^B}{S_3^B}\qquad\text{(B1.5)}$$

in which

$S_1^B=\frac{E_B}{E_C}\frac{1-2\nu_C+\frac{1}{2}(1+\nu_C)R^3/r_2^3}{(1-2\nu_B)\left(R^3/r_2^3-1\right)}$, $S_2^B=-\frac{E_B}{E_A}\frac{1-2\nu_A}{1-2\nu_B}$,

$S_{1^*,2^*}^B=1-2\frac{1-2\nu_B}{1+\nu_B}S_{1,2}^B$ and

$$S_3^B=1-\frac{r_1^3}{r_2^3}+S_1^B\left(1+2\frac{1-2\nu_B}{1+\nu_B}\frac{r_1^3}{r_2^3}\right)-S_2^B\left[\frac{r_1^3}{r_2^3}+2\frac{1-2\nu_B}{1+\nu_B}\left(1-S_1^B\left(\frac{r_1^3}{r_2^3}-1\right)\right)\right].$$

$$e_{rr}^C(r)=-\frac{\varepsilon_1S_1^C+\varepsilon_2S_2^C}{S_4^C}\left(1-\frac{1+\nu_C}{1-2\nu_C}\frac{R^3}{r^3}\right),\qquad\text{(B1.6)}$$

$$e_{\theta\theta}^C(r)=e_{\varphi\varphi}^C(r)=-\frac{\varepsilon_1S_1^C+\varepsilon_2S_2^C}{S_4^C}\left(1+\frac{1}{2}\frac{1+\nu_C}{1-2\nu_C}\frac{R^3}{r^3}\right)\qquad\text{(B1.7)}$$

$$e_{hyd}^C=-3\frac{\varepsilon_1S_1^C+\varepsilon_2S_2^C}{S_4^C},\qquad\text{(B1.8)}$$

where $S_1^C=3\frac{r_1^3}{r_2^3}\frac{1-\nu_B}{1+\nu_B+2(1-2\nu_B)\,r_1^3/r_2^3}$,

$S_2^C=1-2\frac{E_B}{E_A}\frac{(1-2\nu_A)\left(r_1^3/r_2^3-1\right)}{1+\nu_B+2(1-2\nu_B)r_1^3/r_2^3}$, $S_3^C=\frac{1}{2}\frac{1+\nu_C}{1-2\nu_C}\frac{R^3}{r_2^3}+1$

$$S_4^C = S_3^C + \frac{1-S_2^C}{2}\left[\frac{E_C}{E_B}\frac{R^3/r_2^3-1}{1-2\nu_C}\left(\frac{(1+\nu_B)r_1^3/r_2^3+2(1-2\nu_B)}{r_1^3/r_2^3-1}-\frac{E_A}{E_B}\frac{(1+\nu_B)(1-2\nu_B)}{1-2\nu_A}\right)-2S_3^C\right]$$

2) Spherical QD with one shell

$$e_{rr}^A = e_{\theta\theta}^A = e_{\varphi\varphi}^A = \varepsilon_0 S_4^A, \qquad \text{(B2.1)}$$

$$e_{hyd}^A = 3\varepsilon_0 S_4^A, \qquad \text{(B2.2)}$$

where $S_4^A = \left[1+\frac{E_A}{E_B}\frac{(1+\nu_B)R^3/r_0^3+2(1-2\nu_B)}{2(1-2\nu_A)\left(R^3/r_0^3-1\right)}\right]^{-1}$.

$$e_{rr}^B(r) = -\varepsilon_0 S_4^B\left(1-\frac{1+\nu_B}{1-2\nu_B}\frac{R^3}{r^3}\right), \qquad \text{(B2.3)}$$

$$e_{\theta\theta}^B(r) = e_{\varphi\varphi}^B(r) = -\varepsilon_0 S_4^B\left(1+\frac{1}{2}\frac{1+\nu_B}{1-2\nu_B}\frac{R^3}{r^3}\right), \qquad \text{(B2.4)}$$

$$e_{hyd}^B = -3\varepsilon_0 S_4^B, \qquad \text{(B2.5)}$$

where $S_4^B = \left[\frac{1}{2}\frac{1+\nu_B}{1-2\nu_B}\frac{R^3}{r_0^3}+1+\frac{E_B}{E_A}\frac{1-2\nu_A}{1-2\nu_B}\left(\frac{R^3}{r_0^3}-1\right)\right]^{-1}$.

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