Analytical evaluation of strain inside vertical quantum dot stacks

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In this paper the vertical stacks of semiconductor quantum dots (QDs) without dislocations, incorporated in the other semiconductor substrate, for the epitaxial growth in the crystal direction (001) were considered. Analytical expressions for the strain in the both semiconductors were derived for the case when the thicknesses of QDs and the substrate spacers are small enough in comparision with the stack lateral dimensions. In the particular case when the stack consists of InAs QDs in the GaAs substrate, the obtained results were calculated and shown graphically.

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1. Introduction

It was proven many times during the past twenty years that the vertical alignment of the semiconductor QDs into the vertical stacks, is technologically possible [1-4]. This kind of nanostructures could be appropriate for the applications in the semiconductor laser technology [5,6], and for the solar cells fabrication [4].

Until now, there is no published scientific paper about the analytical strain evaluation inside QD stacks. Some of the published papers have discussed results obtained by the numerical methods for the stacks consisted of several QDs [7,8].

In this paper we have generally analised the vertical stacks of the thin cylindrical QDs made of the semiconductor 2, incorporated in the semiconductor 1 substrate. Basic assumptions were: (1) Thicknesses of QDs and spacers much less than the stack lateral dimensions; (2) Coherent crystal growth providing the nanostructure without defects; (3) Both semiconductors with cubic diamond or zinc blende structure; (4) Flat QDs with constant thickness (see Fig. 1), except probably on its lateral edges near the stack side; (5) Arbitrary shape of the horizontal intersection of the stacks.

Because of the assumption (1), the space volume of the stack and surrounding substrate (where the strain varies from its values inside the stack to the zero values in the substrate) is in the very narrow vicinity of the stack side being very small in comparison with the stack volume, and hence its influence could be neglected. Accordingly, there is approximately constant strain inside the QDs, and also another constant strain inside the dots spacers.

2. Analytical evaluation

We have chosen coordinate system $0xyz$ with the z-axis in the crystal direction (001), while the x-axis and the y-axis are in the (100) and (010) crystal directions respectively (see Fig. 1).

Because of the cubic crystal symmetry, for such coordinate system $0xyz$ there would be

$$\varepsilon_{xx} = \varepsilon_{yy}$$
$$\varepsilon_{xy} = \varepsilon_{yz} = \varepsilon_{zx} = 0 \qquad (1)$$

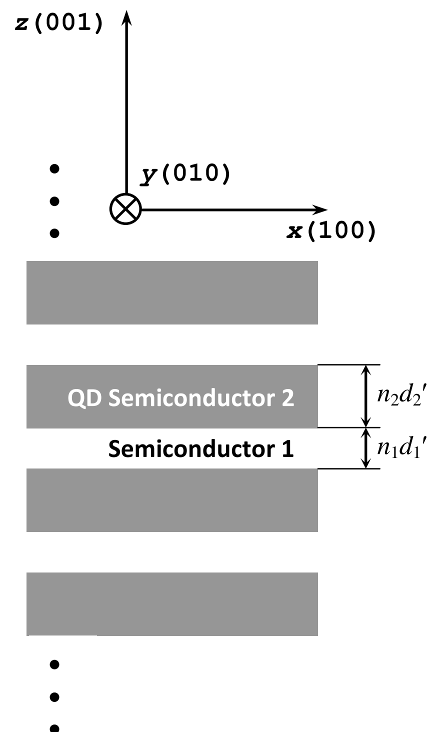

Fig. 1. Semiconductor 2 quantum dot stack in the semiconductor 1 substrate. There is large number of QDs in the stack

Let us designate the transverse strain components as $\varepsilon_p = \varepsilon_{xx} = \varepsilon_{yy}$ and longitudinal strain component as $\varepsilon_n = \varepsilon_{zz}$. Also, let a_1 and a_2 be the unstrained lattice constants of the semiconductors 1 and 2, and a_1' and a_2' their strained values in the xy-plane inside the stack. Because of the coherent crystal growth assumption there would be $a_1' = a_2' = a'$. Accordingly, one gets

$$\varepsilon_{1p} = \frac{a'-a_1}{a_1} = \frac{a'}{a_1} - 1, \quad \varepsilon_{2p} = \frac{a'-a_2}{a_2} = \frac{a'}{a_2} - 1 \quad (2)$$

where ε_{1p} and ε_{2p} are the transverse strain components in the semiconductors 1 and 2.

Let n_1 and n_2 be the numbers of monolayers of the semiconductors 1 and 2 in the stack period, d_1 and d_2 the thicknesses of the unstrained monolayers of the semiconductors 1 and 2, and d_1' and d_2' their strained values. From the coherent growth assumption, it must be the same number of the molecular monolayers in the stack period and the corresponding unstrained surrounding substrate, so it should be:

$$n_1 d_1' + n_2 d_2' = (n_1 + n_2) d_1 \quad (3)$$

Also,

$$\frac{d_1'}{d_1} = \frac{d_1'}{d_1} - 1 + 1 = \frac{d_1' - d_1}{d_1} + 1 = \varepsilon_{1n} + 1$$

and similarly

$$\frac{d_2'}{d_2} = \varepsilon_{2n} + 1$$

After inserting these expressions into eq. (3) one obtains

$$n_1 d_1 (1 + \varepsilon_{1n}) + n_2 d_2 (1 + \varepsilon_{2n}) = (n_1 + n_2) d_1 \quad (4)$$

and

$$\frac{n_1}{n_1 + n_2}(1 + \varepsilon_{1n}) + \frac{n_2}{n_1 + n_2}\frac{d_2}{d_1}(1 + \varepsilon_{2n}) = 1 \quad (5)$$

Because of the same crystal structure, all corresponding geometric parameters of the semiconductors 1 and 2 are proportional, so it would be $\frac{d_2}{d_1} = \frac{a_2}{a_1}$. Accordingly, from eq. (5) one gets

$$(1 - \xi)(1 + \varepsilon_{1n}) + \xi \frac{a_2}{a_1}(1 + \varepsilon_{2n}) = 1 \quad (6)$$

where

$$\xi = \frac{n_2}{n_1 + n_2}$$

The elastic energy density of the cubic crystal is [9,10]:

$$w = \frac{1}{2} C_{11}\left(\varepsilon_{xx}^2 + \varepsilon_{yy}^2 + \varepsilon_{zz}^2\right) + C_{12}\left(\varepsilon_{xx}\varepsilon_{yy} + \varepsilon_{yy}\varepsilon_{zz} + \varepsilon_{zz}\varepsilon_{xx}\right) + 2C_{44}\left(\varepsilon_{xy}^2 + \varepsilon_{yz}^2 + \varepsilon_{zx}^2\right)$$

where C_{ij} are the elastic stiffnesses of that cubic crystal. Because of eq. (1) the single period of the stack has an elastic energy

$$\begin{aligned}\Delta E = w_1 \Delta V_1 + w_2 \Delta V_2 = S n_1 d_1 (1 + \varepsilon_{1n}) \times \\ \times \left[\frac{1}{2} C_{11}^{(1)}\left(2\varepsilon_{1p}^2 + \varepsilon_{1n}^2\right) + C_{12}^{(1)}\left(\varepsilon_{1p}^2 + 2\varepsilon_{1n}\varepsilon_{1p}\right)\right] + \\ + S n_2 d_2 (1 + \varepsilon_{2n}) \times \\ \times \left[\frac{1}{2} C_{11}^{(2)}\left(2\varepsilon_{2p}^2 + \varepsilon_{2n}^2\right) + C_{12}^{(2)}\left(\varepsilon_{2p}^2 + 2\varepsilon_{2n}\varepsilon_{2p}\right)\right]\end{aligned} \quad (7)$$

where w_1 and w_2 are the elastic energy densities in the semiconductors 1 and 2, and ΔV_1 and ΔV_2 are the volumes of single QD and single spacer. According to the principle of minimum energy, the strain values inside the stack could be found from the equations for the minimum of ΔE in subject to eq. (4):

$$\begin{aligned}\frac{\partial}{\partial \varepsilon_{1n}}\left(\Delta E - \beta f(\varepsilon_{1n}, \varepsilon_{2n})\right) = 0 \\ \frac{\partial}{\partial \varepsilon_{2n}}\left(\Delta E - \beta f(\varepsilon_{1n}, \varepsilon_{2n})\right) = 0 \\ \frac{\partial}{\partial a'}\left(\Delta E - \beta f(\varepsilon_{1n}, \varepsilon_{2n})\right) = 0\end{aligned} \quad (8)$$

where β is some constant and

$$f(\varepsilon_{1n}, \varepsilon_{2n}) = n_1 d_1 (1 + \varepsilon_{1n}) + n_2 d_2 (1 + \varepsilon_{2n}) - (n_1 + n_2) d_1$$

After inserting eqs. (4) and (7) into eq. (8), and calculating derivatives, one obtains in the first order approximation:

$$\begin{aligned} S\left[C_{11}^{(1)}\varepsilon_{1n} + \frac{2C_{12}^{(1)}}{a_1}(a' - a_1)\right] - \beta \approx 0 \\ S\left[C_{11}^{(2)}\varepsilon_{2n} + \frac{2C_{12}^{(2)}}{a_2}(a' - a_2)\right] - \beta \approx 0 \\ n_1 \frac{d_1}{a_1}\left[\frac{C_{11}^{(1)} + C_{12}^{(1)}}{a_1}(a' - a_1) + C_{12}^{(1)}\varepsilon_{1n}\right] + \\ + n_2 \frac{d_2}{a_2}\left[\frac{C_{11}^{(2)} + C_{12}^{(2)}}{a_2}(a' - a_2) + C_{12}^{(2)}\varepsilon_{2n}\right] \approx 0 \end{aligned}$$

with assumption that $\varepsilon_{(1;2)n}$ and $\varepsilon_{(1;2)p}$ are small, so the second order terms could be neglected. After eliminating β from the above equations one gets the following system of linear equations, in combination with eq. (6):

$$C_{11}^{(1)}\varepsilon_{1n} - C_{11}^{(2)}\varepsilon_{2n} + 2\left(\frac{C_{12}^{(1)}}{a_1} - \frac{C_{12}^{(2)}}{a_2}\right)a' = 2\left(C_{12}^{(1)} - C_{12}^{(2)}\right)$$

$$\begin{aligned} &(1-\xi)C_{12}^{(1)}\varepsilon_{1n} + \xi C_{12}^{(2)}\varepsilon_{2n} + \\ &+\left[(1-\xi)\frac{C_{11}^{(1)}+C_{12}^{(1)}}{a_1} + \xi\frac{C_{11}^{(2)}+C_{12}^{(2)}}{a_2}\right]a' = \\ &= (1-\xi)\left(C_{11}^{(1)}+C_{12}^{(1)}\right) + \xi\left(C_{11}^{(2)}+C_{12}^{(2)}\right) \end{aligned} \qquad (9)$$

$$(1-\xi)(1+\varepsilon_{1n}) + \xi\frac{a_2}{a_1}(1+\varepsilon_{2n}) = 1$$

From the system of eqs (9), one can obtain longitudinal strain components $\varepsilon_{(1;2)n}$ and a':

$$\varepsilon_{1n} = \frac{D_1}{D},\ \varepsilon_{2n} = \frac{D_2}{D},\ a' = \frac{D_3}{D}$$

where D_i and D are the corresponding determinants of this system of equations. Then transverse strain components $\varepsilon_{(1;2)p}$ can be obtained from eqs. (2).

3. Practical demonstration

In this section we will apply the obtained theoretical results for the case when the stack consists of the InAs QDs incorporated in the GaAs substrate.

Parameters for InAs and GaAs are given in Table 1 [11].

Table 1. InAs, GaAs: Lattice constants and stiffnesses

	Lattice constant:	C_{11} (10^{10}Pa)	C_{12} (10^{10}Pa)	C_{44} (10^{10}Pa)
GaAs	5.6533 Å	11.88	5.38	5.94
InAs	6.0583 Å	8.329	4.526	3.959

After inserting these parameters in the system of eqs. (9), and solving the system one gets:

$$\begin{aligned} \varepsilon_{1n} &= \frac{-0.1810\xi^2 + 1.0583\xi}{\xi^2 - 1.4412\xi - 7.0792} \\ \varepsilon_{2n} &= \frac{-0.2357\xi^2 + 1.2528\xi - 0.5143}{\xi^2 - 1.4412\xi - 7.0792} \\ a' &= \frac{4.6303\xi^2 - 11.2424\xi - 40.0207}{\xi^2 - 1.4412\xi - 7.0792}[\text{nm}] \end{aligned} \qquad (10)$$

while strains $\varepsilon_{(1;2)p}$ can be calculated according to eqs. (2):

$$\begin{aligned} \varepsilon_{1p} &= \frac{-0.1810\xi^2 - 0.5475\xi}{\xi^2 - 1.4412\xi - 7.0792} \\ \varepsilon_{2p} &= \frac{-0.2357\xi^2 - 0.4145\xi + 0.4732}{\xi^2 - 1.4412\xi - 7.0792} \end{aligned} \qquad (11)$$

Using eqs. (10) and (11) strain graphs are plotted in Figs. 2 and 3.

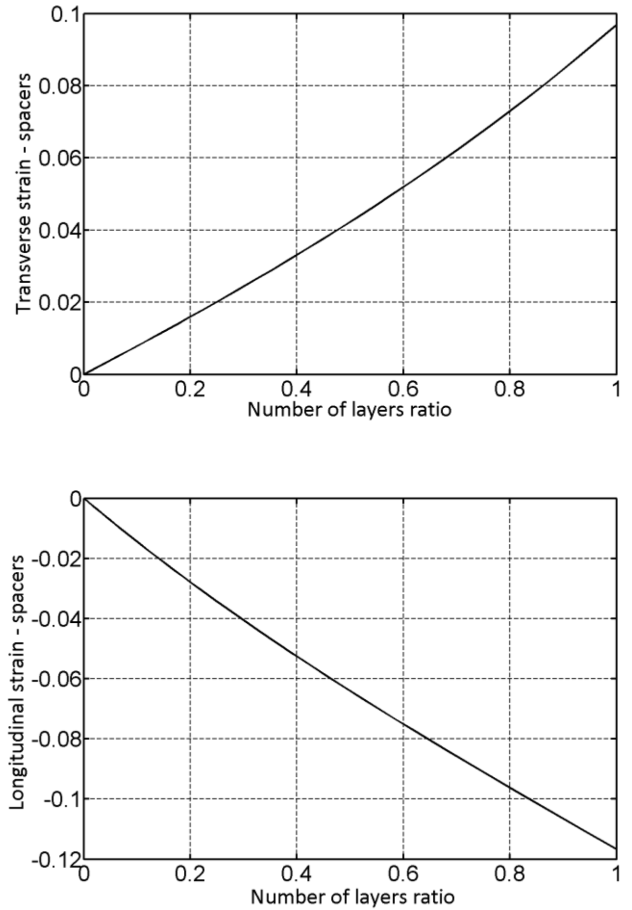

Fig. 2. Transverse and longitudinal strains in the GaAs spacers. The transverse strain in the spacer is always positive and varies in the interval $0 \le \varepsilon_{1p} \le 9.69\%$, while the longitudinal strain in the GaAs spacer is always negative and varies in the interval $-11.67\% \le \varepsilon_{1n} \le 0$.

It is well known how the mechanical strain affects the electronic and optical properties of the semiconductor [12]. Pretty large obtained strain variation in QDs could moderately affect their electronic and optical properties. The mechanical strain varies smoothly with ratio ξ between the number of monolayers in QDs and number of monolayers in the stack period, so the electronic and optical properties of this nanostructure could be precisely controlled by changing the value of ξ.

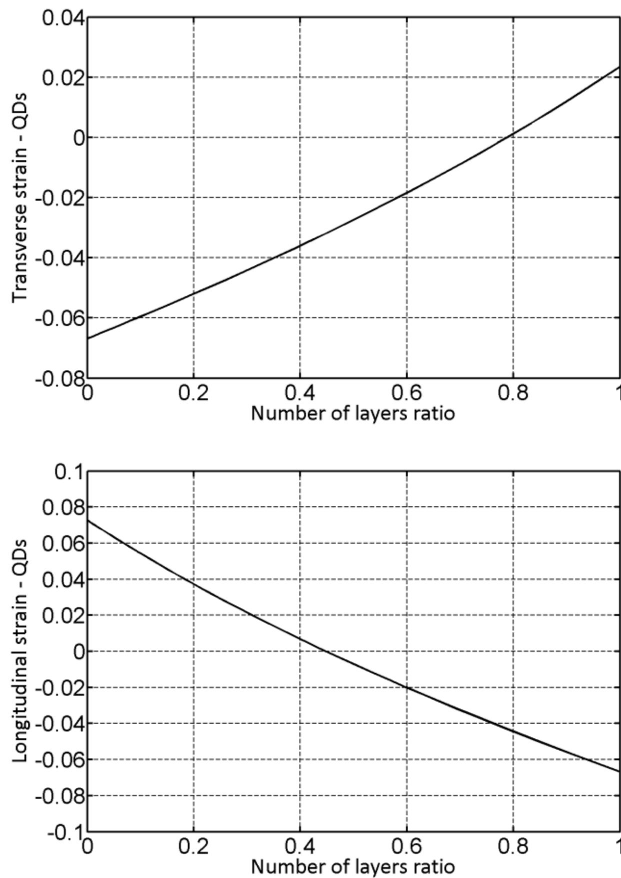

Fig. 3. Transverse and longitudinal strains in InAs QDs. The QDs transverse strain ε_{2p} varies in the interval $-6.68\% \le \varepsilon_{2p} \le 2.35\%$ and changes sign from negative to positive for $\xi \approx 0.778$, while the QDs longitudinal strain ε_{2n} varies in the interval $-6.68\% \le \varepsilon_{1n} \le 7.27\%$ and changes sign from positive to negative for $\xi \approx 0.448$.

4. Conclusions

In this paper we have derived the approximate analytical expressions for the strain inside the QDs stack. The stack of semiconductor 2 cylindrical QDs was adopted, separated by the semiconductor 1 substrate spacers, for the most common (001) direction of the crystal growth. The same cubic crystal stucture was supposed for both semiconductors. These expressions were derived from the boundary conditions between QDs and the substrate. First boundary conditions were chosen for the cross section plane of the stack, while the second boundary conditions were chosen for the stack side. Basic assumption was the crystal growth without dislocations.

The obtained results were applied in the case of the InAs QDs and the GaAs substrate. All strains have been calculated and graphically presented in respect to the ratio ξ between the number of monolayers in QDs and number of monolayers in the stack period. Both cross-section transverse strain and stack axis longitudinal strain in QDs change sign with changing ξ. For thinner QDs biaxial cross-section stress dominates, e.g. QDs compress in their cross sections and stretch in the axial direction. For thicker QDs, the uniaxial stack side stress dominates, e.g. QDs stretch in their cross sections and compress in the axial direction.

The QDs transverse strain varies with ξ in the interval $-6.68\% \le \varepsilon_{2p} \le 2.35\%$, while the axial strain varies in the interval $-6.68\% \le \varepsilon_{1n} \le 7.27\%$. Such a large strain values, which result from the lattice constants mismatch, could not be practically reached by means of the external forces, because they far exceed the cracking value.

Due to the strain variation inside QDs in the stack, their electronic and optical properties could be precisely controlled by the ratio ξ.

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