Modeling of crystal growth in heteroepitaxial systems

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Abstract. This paper investigates the elastic deformation of the structure containing InAs nanoclusters in a pyramid, grown on the substrate GaAs. So far the data have not been grown quantum dots (QDs), one of the reasons is significant difference of periods, which reaches 7%. Ideally atomic plane on the border of QDs and substrate must continuously sews. Due to the difference in lattice periods crosslinking occurring deformations and mechanical stresses, the magnitude of which is proportional to the number of atomic planes, the size of base of the pyramid. Therefore, when you reach a certain size islands (quantum dots), they may experience mechanical stresses p_{cr} sufficient for the appearance of structural defects - dislocations, fractures.

1. Introduction.

One of the methods of forming quantum dots is based on semiconductor nanostructures self organization during its epitaxial growth [1]. Mechanical stresses in epitaxial film of future quantum dot (QD) material and in its islands on the surface of the substrate are critical in the transition from the film's growth to growth of islets (Stranski-Krastanov mechanism [2,3]).These stresses are important in the further growth of QD in size, changing of its shape and its distribution on the substrate. Notable among material for QD occupies the binary semiconductors of the $A^{III}B^{V}$ family such as InAs, InSb [4]. The problem for the cultivation of such QD is the absence of complementary substrates with a close lattice period. Thus, the lattice mismatch periods in QD and in the coming per period substrate for InAs/GaAs system equals to about 7%, and for InSb/GaAs system – 14.5% [4,5]. As a result, in the QD-substrate interface there are occurred the mechanical stresses and deformations, the magnitude of which increases with the number of cross-linked atomic planes of that fundamental size of QD, which is often the pyramid . Therefore, when one reaches a certain size of QD, then the mechanical stresses p_{cr} appear, the value of which is sufficient for the appearance of structural defects namely – fractures, dislocations, etc. [5,6].

In this regard there is still the urgent task to find the mechanical stresses and deformations in InAs/GaAs systems and to estimate the size of QD, the achievement of which in the process of growth process there is running the conditions for the formation of structural defects. It is divided into two tasks: *i)* to find the stresses and deformations occurred in the InAs/GaAs heteroepitaxial system; *ii)* to obtain an estimate of the size of the QD the achievement of which there are appeared the mechanical stresses sufficient for the formation of defects.

2. The calculation of stresses in the InAs/GaAs system.

2.1.Issue formation.

Let's consider the InAs/GaAs heteroepitaxial system of two binary semiconductors in the vicinity of the QD/substrate interface − figure 1. We assume that QD of InAs has the shape of a square pyramid with bases in length l and height h . The QD base's length and height are linked with its growth on a substrate particularly due Wolf-Cashew theorem [7]. InAs and GaAs crystals belong to point group symmetry of $\bar{4}3m$ cubic system (sphalerite-type structure). Also consider that the pieces of QD atomic planes formed one over another from the interface will be a square, their orientation is (001) and the next size is smaller than the previous – see figure 1. If each upper QD atomic plane is

shorter than the previous one from both edges (as is when atoms in planes are strictly one above the other), in this case it should be realized the condition $l = na$ where n – pairwise, a – InAs lattice period and then we receive $h = l/2$ where h – the height of the pyramid l – the length of the base of the pyramid. The sides of the base are oriented along the crystallographic axes [010] and in $x = \pm l/2$ and $y = \pm l/2$ [100]. The sides of the pyramid has the orientation (010). The substrate is represented as the parallelepiped of sizes $L_x, L_y, L_z >> h$. The beginning of the coordinate system and its axis were chosen due to figure 1.

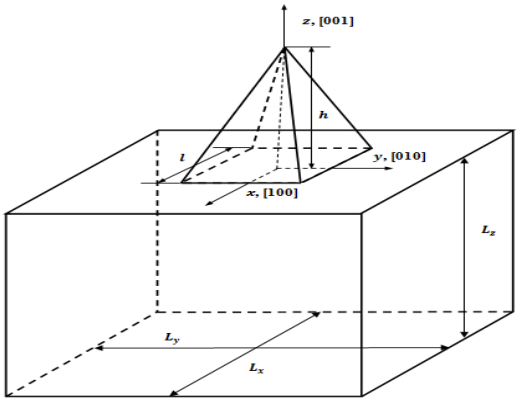

Figure 1. Schematic representation of the piece of substrate (a parallelepiped) and quantum dots (a pyramid) for the system InAs/GaAs

Considering the elastic properties of the system, we will not take its full account of atomic structure, despite the fact that QD as well as substrate contains thousands of atoms. QD for instance shown at figure 1, at $n = 20$ contains 1 771 atoms [8]. This assumption can consider the system as a complete environment. We also believe that as a zero approximation for the deformation description in the system can be applied the linear theory of elasticity.

Within these assumptions the stresses are satisfied with the Lame equation:

$$\frac{\partial p_{ij}}{\partial x_j} = 0 \tag{1}$$

where p_{ij} – (mechanical stress tensor for anisotropic linear environment is given by Hooke's law:

$$p_{ij} = C_{ijkl} u_{kl}, \tag{2}$$

where C_{ijkl} – elastic constants tensor of environment, strain tensor is defined as $2u_{kl} = \partial_l u_k + \partial_k u_l$, deformation vector $\vec{u} = u_x \vec{e}_x + u_y \vec{e}_y + u_z \vec{e}_z$, and ∂_k is partial to coordinate x_k.

GaAs and InAs semiconductor crystals have the same symmetry point group so their elasticity tensors in matrix representation has the same form [9]:

$$C_{ijkl} = \begin{pmatrix} C_{11} & C_{12} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{11} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{12} & C_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{44} \end{pmatrix} \tag{3}$$

and their value and periods of crystalline structure for GaAs and InAs are shown in Table 1 taken from [9].

Table 1. Modules of elastic constants and lattice period

	InAs	GaAs
$C_{11}(Pa)$	$8,34\times10^{10}$	$1,19\times10^{11}$
$C_{12}(Pa)$	$4,54\times10^{10}$	$5,34\times10^{10}$
$C_{44}(Pa)$	$3,95\times10^{10}$	$5,96\times10^{10}$
a (nm)	0.605886	0.565321

Data shown shows GaAs period is 7% at the InAs period still the modulus of elasticity is about 15-33% higher. This means that at one and the same deformation tensor u_{kl} on both sides of the interface the QD-substrate in the substrate system there can be more mechanical loads. Similarly, under the same mechanical loads p_{ij} on both sides of the interface in the QD material there can appear larger relative deformation. From a physical point of view, on the both sides of the interface of deformation and mechanical stresses should be continuous. Therefore, detailed answer to the issue concerning deformations and stresses in the system should be due to the equations (1,2) with clear view of the tensor C_{ijkl} due (3) and the values of elasticity coefficients due Table 1.

2.2. Mathematical model

2.2.1.Equation. For isotropic elastic environment the metric representation of tensor has the form [10]:

$$C_{ijkl}^{isotr}=\begin{pmatrix}\lambda+2\mu & \lambda & \lambda & 0 & 0 & 0\\ \lambda & \lambda+2\mu & \lambda & 0 & 0 & 0\\ \lambda & \lambda & \lambda+2\mu & 0 & 0 & 0\\ 0 & 0 & 0 & \mu & 0 & 0\\ 0 & 0 & 0 & 0 & \mu & 0\\ 0 & 0 & 0 & 0 & 0 & \mu\end{pmatrix}, \quad (4)$$

where λ and μ – Lame parameters while Hooke's law is :

$$p_{ij}=\lambda\delta_{ij}div\vec{u}+2\mu u_{ij}. \quad (5)$$

The structure of the matrix (3) and (4) is the same that is why for assessing of elastic constants tensor deviations for GaAs and InAs from tensor for isotropic environment we will choose the following value:

$$\delta=\left|\frac{C_{12}+C_{44}-C_{11}}{C_{11}}\right|,$$

which is zero for isotropic environment. Due to Table 1 it is followed that for InAs $\delta\approx0.02$, and for GaAs $\delta\approx0.05$. These values are somewhat smaller than the non-complementarity lattices and significantly less than the relative deviation of the elastic modules of its crystals.

So we make the third step: the deformations in QD-substrate we will describe with the equations of elasticity theory for two isotropic environments. Then the equation (1, 2) takes the form of:

$$(\lambda+\mu)\vec{\nabla}div\vec{u}+\mu\Delta\vec{u}=0, \quad (6)$$

where Lame parameters are expressed through the matrix coefficients of elastic constants as $\lambda=C_{12}$, $\mu=C_{44}$ on the both parts of the QD-substrate system and its value can be found in the Table 1.

2.2.2. Boundary conditions. As Lame parameters in the equation (6) are piecewise continuous, and their solutions describe continuous deformations than the terms of their will build according to the fact that in a perfect defect-free quantum dot electrons move in a continuous crystalline potential. It is necessary that GaAs and InAs atomic planes continuously without spaces pass one another. This

condition is met if the atomic planes of InAs and GaAs crystal lattice are oriented in the same crystallographic direction and deformed without altering the symmetry.

Figure 2 a) it is shown the fragment of QD-substrate geometric contact where the atomic planes [010] in QD and in the substrate (see the figure 1) are shown as the vertical lines. Here due to our choice are stitched only average atomic planes. On the figure 2 b) is shown the same fragment where formally and without gaps all atomic planes are stitched. The average planes of both environments haven't been displaced and the displacement of other planes is increasing together with its distance from the axis of the system. Under such terms the mechanical stresses will increase around the interface. At some distance from the axis of the system they can reach such values when it is energetically favorable to pass the part of atomic plane near the interface. It can lead to structural defect – figure 2c).

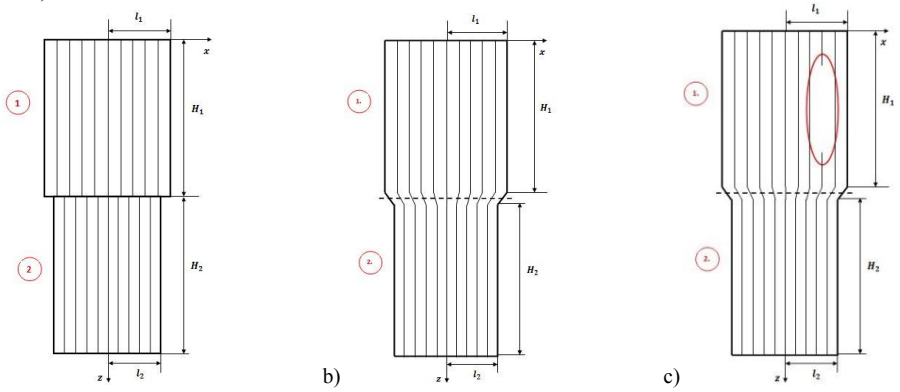

Figure 2. Scheme of atomic planes crosslinking [010] (vertical line) in QD (1, top) and in the substrate (2, below) while its contact in the plane $z=0$: a) geometric contact; b) stitching starting from the central plane; c) stitching of atomic planes with the passing of one of it.

Based on these considerations, we will construct a crosslinking conditions at the interface. The first follows from the z-component conditional continuity of vector deformation under normal passing through the interface's plane along each atomic plane [010] with the same number $n=0,\pm1,\ldots$ that is counted from the average atomic plane in figure 2 a). A similar condition is fair along the atomic planes as well [100]. So $u_z^{(1)}\left(na_1,ka_1,z=+0\right)=u_z^{(2)}\left(na_2,ka_2,z=-0\right)$ where $k=0,\pm1,\ldots$. If the axis of coordinate system Oz combines with an average atomic plane, axis Ox, Oy direct due to the figure 1, then for the $u_z^{(1,2)}\left(x,y,z\right)$ on the verge of a square QD and substrate obtain the following homogeneous boundary conditions:

$$u_z^{(1)}\left(x,y,0\right)=u_z^{(2)}\left(\alpha x,\alpha y,0\right), \qquad (7)$$

where the coordinates $x,y\in\left[-l_1,l_1\right]$ are within the QD foundations and multiplier $\alpha=l_2/l_1$ in the arguments of deformations in substrate appears due to the fact that for the same number of atomic planes N in QD and substrate their lateral dimensions $l_{1,2}=Na_{1,2}$ will be different due to different lattice periods $a_1>a_2$,due to the Table 1.

The second and third conditions set continuity of nuclear axes of which are formed the atomic planes in QD and in the substrate while the normal passing through the interface along each of these axes. So we get the following correlation :

$$na_1+u_x^{(1)}\left(na_1,ka_1,z=+0\right)=na_2+u_x^{(2)}\left(na_2,ka_2,z=-0\right),$$
$$ka_1+u_y^{(1)}\left(na_1,ka_1,z=+0\right)=ka_2+u_y^{(2)}\left(na_2,ka_2,z=-0\right).$$

If now to move to continuous coordinates we obtain the following inhomogeneous boundary conditions for transverse vector components of deformation in a plane of interface:

$$\begin{aligned} x + u_x^{(1)}(x, y, z = +0) &= \alpha x + u_x^{(2)}(\alpha x, \alpha y, z = -0), \\ y + u_y^{(1)}(x, y, z = +0) &= \alpha y + u_y^{(2)}(\alpha x, \alpha y, z = -0). \end{aligned} \tag{8}$$

The outside sides of QD and the substrate will be assumed as free, so they just of homogeneous boundary conditions

$$p_{ij} n_j \big|_S = 0. \tag{9}$$

We believe that to the QD-substrate system there is not attached the external forces. But the boundary condition (8) is not uniform and it causes the appearance of deformations and stresses in the system with no complementary QD and substrate. It emerged as a result of the conditions of continuity of atomic planes in the system. Provided $a_1 = a_2$ we get $\alpha = 1$ and then conditions (7,8) indicate that the system has the homocrossing. That the substrate and QD grown on it has the same chemical composition or similar symmetry and steel lattice.

2.2.3. Solution of equations. In the QD-substrate system there is no internal sources for the emergence of deformations except the interface so one can introduce the vector displacement such as

$$\vec{u}(x, z) = \vec{\nabla} \psi(x, z), \tag{10}$$

where $\psi(x, y)$ is arbitrary scalar function. Substitute (10) into the equation (6) and obtain the equation of the third order $(\lambda + 2\mu)\vec{\nabla}\Delta\psi(x, z) = 0$. Its solution as a single integral is easy to be found $\Delta\psi(x, z) = \vec{C}$, a solution of this equation is the sum of the general solution of homogeneous equation and the particular solution of inhomogeneous equation.

Since the boundary conditions for ψ -functions arising from (7-10) have the form of conditions for the second derivatives so heterogeneous solution will not give a contribution to the full solution of equations. So put constant $C = 0$. Get the Laplace equation $\Delta\psi(x, z) = 0$.

Using the Lame's equation (6) and above assumptions formulated the components of vector displacement can be found in both environments.

$$u_x^{(1)}(x, z) = \sum_n \tilde{D}_n^{(1)}\left(-k_n^{(1)}\right) \mathrm{sh} k_n^{(1)} z \sin k_n^{(1)} x, \tag{11a}$$

$$u_z^{(1)}(x, z) = \sum_n \tilde{D}_n^{(1)} k_n^{(1)} \mathrm{ch} k_n^{(1)} z \cos k_n^{(1)} x, \tag{11b}$$

$$u_x^{(2)}(x, z) = \sum_n \tilde{D}_n^{(2)}\left(-k_n^{(2)}\right) \times \left(\mathrm{sh} k_n^{(2)} z - \mathrm{th} k_n^{(2)} H_2 \mathrm{ch} k_n^{(2)} z\right) \sin k_n^{(2)} x, \tag{11c}$$

$$u_z^{(2)}(x, z) = \sum_n \tilde{D}_n^{(2)} k_n^{(2)} \times \left(\mathrm{ch} k_n^{(2)} z - \mathrm{th} k_n^{(2)} H_2 \mathrm{sh} k_n^{(2)} z\right) \cos k_n^{(2)} x. \tag{11d}$$

where $u_{x,z}^{(1,2)}(x, z)$ – the components of vector displacement in both environments.

Due to the Hooke's law the components of mechanical stresses will be written through the deformation:

$$p_{xx}^{(1)}(x, z) = C_{11}^{(1)} u_{xx}^{(1)} + C_{12}^{(1)} u_{zz}^{(1)}, \tag{12a}$$

$$p_{zz}^{(1)}(x, z) = C_{11}^{(1)} u_{zz}^{(1)} + C_{12}^{(1)} u_{xx}^{(1)}, \tag{12b}$$

$$p_{xx}^{(2)}(x, z) = C_{11}^{(2)} u_{xx}^{(2)} + C_{12}^{(2)} u_{zz}^{(2)}, \tag{12c}$$

$$p_{zz}^{(2)}(x, z) = C_{11}^{(2)} u_{zz}^{(2)} + C_{12}^{(2)} u_{xx}^{(2)}, \tag{12d}$$

where $u_{xx}^{(1,2)} = \dfrac{\partial u_x^{(1,2)}}{\partial x}$, $u_{zz}^{(1,2)} = \dfrac{\partial u_z^{(1,2)}}{\partial z}$ – the deformation of components.

So we have got the deformations and stresses in the model of QD-substrate that allows us to assess of heir depending on the linear dimensions of quantum dots on the interface.

3. Results and discussion

3.1. Numerical calculations. The analytical estimates and calculations are supplemented with the numerical calculations in the work. We are considering the model of QD-substrate in which the lateral dimensions of substrate are much larger than the QD's dimensions which has the triangular cross section. In the longitudinal direction the system is infinite so the two-dimensional case is considered – figure 3.

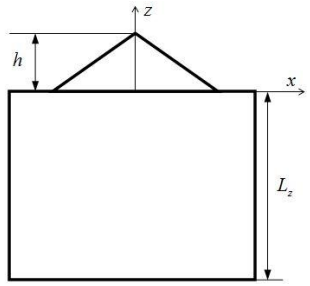

Figure 3. Model quantum dots on a substrate

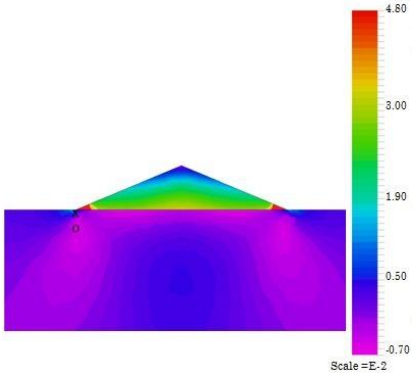

Figure 4. z -component of mechanical stresses

Equation (6) for the deformation together with the boundary conditions on the interface and the outside of the system (7-9) are solved numerically using FlexPDE.

In figure 4 it is shown the z -component of mechanical stresses. We emphasize that within the tops of the foundations the mechanical tensions reach its maximum value. In turn, this will be the most likely QD area for the appearance of dislocations.

4.Conclusion

1. It has been established at the ideal stitching of atomic QD planes and substrates the only source of mechanical stresses and deformations is a mismatch of lattice period.
2. Analytical estimates and numerical calculations show that the maximum stresses in the system occur at the edges of QD-substrate interface, so there will be created conditions for the emergence of defects.
3.The maximum tension of elastic modulus QD order scans occur when its transverse size up to several tens of periods in the event that non-period lattice gratings is about 7%

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