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The Conditions of Formation of the Uniform-Sized Quantum Dots in the Field of an Ultrasonic Wave

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Abstract. The non-linear diffusion-deformation theory of self-organization of nanoclusters of dot defects in semiconductor exposed to ultrasound treatment that considers the interaction of defects among themselves and with atoms of a matrix via the elastic field created by dot defects and an acoustic wave is developed. Within this theory the influence of ultrasound on the conditions of formation of spherical nanoclusters and their radius is investigated. The nanocluster size depending on average concentration of defects and amplitude of an acoustic wave is determined. It is established that ultrasonic treatment of the semiconductor in the process of formation of an ensemble of nanoclusters leads to reduction of dispersion of their sizes. In the framework of this model, a possibility of the ultrasound-stimulated the size dispersion reduction of strained InAs/GaAs quantum dots doped with an isovalent impurity are analyzed.

Introduction

In recent years, a new approach to controlling the properties of semiconductor quantum dot (QD) heterostructures has been developed. The approach is based on the introduction of a single impurity atom into a QD [1]. This problem is prospective for present day optoelectronics, specifically, for the production of single electron devices that may find application is quantum computers [2]. Progress in the development of nanotechnology and the physics of nanostructures has led to the practical implementation of various types of optoelectronic devices based on InAs QD arrays on wide gap GaAs substrates [3 – 6]. One of the ways of forming ordered QD arrays is via the self assembly of QDs on the crystal surface. The kinetics of epitaxial growth and the distribution of strains in the QD – matrix system influence the QD size, shape, and arrangement in the matrix [6 – 8]. The extraordinary properties of QD structures reveal themselves, only if the QDs are as uniform in size and shape as possible and the QD array is of high density (about 10^{11} cm^{-2}).

Therefore, the main problem in growing QDs is to control their morphology: the average size, density, uniformity, etc. All of these QD characteristics can be controlled by varying the technological parameters of the growth process [9 – 11].

In Ref. [12, 13], it was found experimentally that the introduction of nitrogen [13] and bismuth [12] impurities considerably improves the optical properties of InAs/GaAs QDs. In Ref. [7], the theory of deformation was developed for QDs doped with an isovalent impurity. The theory explained experimental data on the creation of an array of uniform InAs QDs doped with Bi [12]. Bismuth is not an electrically active impurity, i.e. it does not increase the charge carrier concentration. However, it substantially changes the conditions of QD formation owing to the induced diffusion-deformation flux. The direction of an atomic flux is governed by signs of the deformation potential and the strain gradient. In other words, defects that play the role of stretching centres are accumulated in the region with a relative stretching deformation of the material, whereas defects that are squeezing centres are accumulated in the region with the relative squeezing deformation. Since the covalent radius of In is larger than that of Ga, In atoms can be regarded as stretching centres. The Bi impurity is also a stretching centre.

Therefore, the deformation-induced flux of In atoms promotes their localization in the QDs, which, accordingly, leads to the restriction of their migration mobility and to a higher uniformity of

QD sizes. Evidently, the creation of a non-uniform deformation by an ultrasonic wave at the growth of InAs/GaAs QD with an impurity induces additional deformation fluxes of In atoms, which would result in their higher localization in the QDs, provided a proper choice of corresponding parameters [14 – 16].

The non-linear diffusion-deformation theory of self-organization of nanoclusters of dot defects in semiconductor exposed to ultrasound treatment that considers the interaction of defects among themselves and with atoms of a matrix via the elastic field created by dot defects and an acoustic wave is developed. Within this theory the influence of ultrasound on the conditions of formation of spherical nanoclusters and their radius is investigated.

Model

Let's consider the spherically symmetric defect crystal system in which centre ($r = 0$) as a result of non-linear interaction of defects in the elastic field the cluster of these defects is formed. Let's allocate the spherical area of the crystal with radius $R_0 >> l_d$, where l_d is the average free path length of defect.

The potential energy of elastic interaction of defect can be presented in the form:

$$U_i = U_{dd}^{\text{int}} + U_{da}^{\text{int}}. \tag{1}$$

Here the first term $U_{dd}^{\text{int}} = -\frac{2}{3} K \frac{1-2\nu}{1-\nu} N \Delta\Omega_d^2$ is the energy of defects interaction among themselves, and the second term $U_{da}^{\text{int}} = -K\varepsilon(r)\Delta\Omega_d - K r_{da}^2 \Delta\Omega_d \, \partial^2\varepsilon(r)/\partial r^2$ is the energy of defect interaction with matrix atoms, where K is an elasticity coefficient; ν is the Poisson coefficient; $N(r)$ is the defects concentration; $\Delta\Omega_d$ is the crystalline volume change by one defect; $\varepsilon_{rr}(r) = \varepsilon(r)$ is a strain tensor radial component; r_{da} is the characteristic length of interaction between the defect and matrix atoms.

The elastic field of a solid influence on the defect with the force: $\mathbf{F} = -\mathbf{grad} U_i$. Under this force, the defects in the elastic field get the velocity:

$$\mathbf{\upsilon} = \mu\mathbf{F} = \frac{DK}{k_B T} \mathbf{grad} \left(\frac{2}{3} \frac{1-2\nu}{1-\nu} N(r) \Delta\Omega_d^2 + \varepsilon(r)\Delta\Omega_d + \frac{\partial^2 \varepsilon(r)}{\partial r^2} r_{da}^2 \Delta\Omega_d \right), \tag{2}$$

where μ, D are the mobility and diffusion coefficient of defects; T is the temperature; k_B is the Boltzmann constant. Here we use the Einstein relation to determine the impurity mobility.

As we can see from (2), the defects in the elastic field get the velocity is determined by the deformation gradients and crystal volume gain due to these defects.

Taking (2) into account, the stationary flow of defects can be presented as

$$j = -D \frac{\partial N}{\partial r} + N \frac{DK\Delta\Omega_d}{k_B T} \left(\frac{2}{3} \frac{1-2\nu}{1-\nu} \frac{\partial N}{\partial r} \Delta\Omega_d + \frac{\partial \varepsilon}{\partial r} + \frac{\partial^3 \varepsilon}{\partial r^3} r_{da}^2 \right). \tag{3}$$

The potential energy density of the elastic defects-free continuum taking into account the anharmonic components can be presented as

$$U_a = K\left(\varepsilon^2/2 + \alpha\varepsilon^3/3 + \beta\varepsilon^4/4 + a_0^2 \varepsilon \, \partial^2\varepsilon/\partial r^2\right), \tag{4}$$

where α, β are the elastic anharmonicity constants; a_0 is the characteristic distance of the crystalline matrix atoms interaction that is roughly equal to the matrix lattice parameter.

Then, taking into account (1) and (4), free energy density of the crystal with defects can be presented as:

$$\Phi = U_a + NU_i - TS = K\left(\varepsilon^2/2 + \alpha\varepsilon^3/3 + \beta\varepsilon^4/4 + a_0^2\varepsilon\,\partial^2\varepsilon/\partial r^2 - \frac{1}{3}\frac{1-2\nu}{1-\nu}N^2(r)\Delta\Omega_d^2 - \right.$$
$$\left. - N(r)\varepsilon(r)\Delta\Omega_d - N(r)\frac{\partial^2\varepsilon(r)}{\partial r^2}r_{da}^2\Delta\Omega_d \right) - TS\,, \tag{5}$$

where S is the entropy density.

Applying the relation $\sigma = \frac{\partial\Phi}{\partial\varepsilon}$, we obtain the mechanical stress expression:

$$\sigma = K\left(\varepsilon + \alpha\varepsilon^2 + \beta\varepsilon^3 + a_0^2\frac{\partial^2\varepsilon}{\partial r^2} - \frac{2}{3}\frac{1-2\nu}{1-\nu}N\frac{\partial N}{\partial\varepsilon}\Delta\Omega_d^2 - \right.$$
$$\left. - N\Delta\Omega_d - \frac{\partial N}{\partial\varepsilon}\varepsilon(r)\Delta\Omega_d - \frac{\partial N}{\partial\varepsilon}\frac{\partial^2\varepsilon(r)}{\partial r^2}r_{da}^2\Delta\Omega_d \right). \tag{6}$$

The mechanical stress in an ultrasonically treated solid, subject to the anharmonic components, is

$$\tilde{\sigma} = \sigma + K\varepsilon_0\cos\omega t + K\alpha(\varepsilon_0\cos\omega t)^2 + K\beta(\varepsilon_0\cos\omega t)^3\,, \tag{7}$$

where ε_0 is an ultrasonically induced deformation amplitude. Here the wave length $\lambda >> R_0$. Averaging by the time, we obtain:

$$\tilde{\sigma} = K\left(\varepsilon + \tilde{\alpha}\varepsilon^2 + \beta\varepsilon^3 + a_0^2\frac{\partial^2\varepsilon}{\partial r^2} - \frac{2}{3}\frac{1-2\nu}{1-\nu}N\frac{\partial N}{\partial\varepsilon}\Delta\Omega_d^2 - \right.$$
$$\left. - \Delta\Omega_d\left(N - \frac{\partial N}{\partial\varepsilon}\varepsilon(r) - \frac{\partial N}{\partial\varepsilon}\frac{\partial^2\varepsilon(r)}{\partial r^2}r_{da}^2 \right) \right), \tag{8}$$

where $\tilde{\alpha} = \alpha(1 + \frac{\varepsilon_0^2}{2\varepsilon^2})$.

From the strained solid equilibrium condition $\frac{\partial\tilde{\sigma}}{\partial r} = 0$ we obtain the following deformation equation:

$$\frac{\partial\varepsilon}{\partial r}\left(1 - \frac{\partial N}{\partial\varepsilon}\Delta\Omega_d\right) + \tilde{\alpha}\frac{\partial(\varepsilon^2)}{\partial r} + \beta\frac{\partial(\varepsilon^3)}{\partial r} + \frac{\partial^3\varepsilon}{\partial r^3}\left(a_0^2 - \frac{\partial N}{\partial\varepsilon}r_{da}^2\Delta\Omega_d\right) -$$
$$\frac{\partial N}{\partial r}\left(\frac{2}{3}\frac{1-2\nu}{1-\nu}\frac{\partial N}{\partial\varepsilon}\Delta\Omega_d^2 + \Delta\Omega_d\right) = 0\,. \tag{9}$$

Taking into account (3), the diffusion steady-state equation for defects can be written as:

$$\mathrm{div}\left[D\frac{\partial N}{\partial r} + N\frac{DK\Delta\Omega_d}{k_BT}\left(\frac{2}{3}\frac{1-2\nu}{1-\nu}\frac{\partial N}{\partial r}\Delta\Omega_d + \frac{\partial\varepsilon}{\partial r} + \frac{\partial^3\varepsilon}{\partial r^3}r_{da}^2\right)\right] + G_d - \frac{N_d}{\tau_d} = 0\,, \tag{10}$$

where G_d, τ_d are the generation rate and defect lifetime, respectively.

Let us present the defect concentration and deformation as

$$N_d(r) = N_1(r) + N_0, \tag{11}$$

$$\varepsilon(r) = \varepsilon_1(r) + N_0\Delta\Omega_d, \tag{12}$$

where $N_1(r)$, $\varepsilon_1(r)$ are the space inhomogeneous components of defects concentration and deformation, respectively; $N_1(r) << N_0$, $\varepsilon_1(r) << N_0\Delta\Omega_d$.

Thus, $\widetilde{\alpha} = \alpha\left(1 + \dfrac{\varepsilon_0^2}{2\left(N_0\Delta\Omega_d\right)^2 + \varepsilon_0^2}\right)$.

Substituting (11), (12) into (9), (10), taking into account that $N_1(r) << N_0$ and at $r \to R_0$ the conditions $\dfrac{\partial N_1}{\partial r} = 0$ and $\dfrac{\partial \varepsilon_1}{\partial r} = 0$ must be kept, we obtain that $N_0 = G_d\tau_d$ and the equation for $N_1(r)$ and $\varepsilon_1(r)$:

$$\frac{\partial N_1}{\partial r} - \frac{N_0 K\Delta\Omega_d}{k_B T}\left(\frac{2}{3}\frac{1-2\nu}{1-\nu}\frac{\partial N_1}{\partial r}\Delta\Omega_d^2 + \frac{\partial \varepsilon_1}{\partial r} + \frac{\partial^3 \varepsilon_1}{\partial r^3}r_{da}^2\right) = 0, \tag{13}$$

$$\begin{aligned}&\frac{\partial \varepsilon_1}{\partial r}\left(1 - \frac{\partial N_1}{\partial \varepsilon_1}\Delta\Omega_d\right) + \widetilde{\alpha}\left(2N_0\Delta\Omega_d\frac{\partial \varepsilon_1}{\partial r} + \frac{\partial\left(\varepsilon_1^2\right)}{\partial r}\right) + \\ &+ \beta\left(3\left(N_0\Delta\Omega_d\right)^2\frac{\partial \varepsilon_1}{\partial r} + 3N_0\Delta\Omega_d\frac{\partial\left(\varepsilon_1^2\right)}{\partial r} + \frac{\partial\left(\varepsilon_1^3\right)}{\partial r}\right) + \\ &+ \frac{\partial^3 \varepsilon_1}{\partial r^3}\left(a_0^2 - \frac{\partial N_1}{\partial \varepsilon_1}r_{da}^2\Delta\Omega_d\right) - \frac{\partial N_1}{\partial r}\left(\frac{2}{3}\frac{1-2\nu}{1-\nu}\frac{\partial N_1}{\partial \varepsilon_1}\Delta\Omega_d^2 + \Delta\Omega_d\right) = 0.\end{aligned} \tag{14}$$

Integrating the equation (13), we obtain:

$$N_1 = \frac{1}{\Delta\Omega_d}\frac{N_0/N_c}{1 - \dfrac{2}{3}\dfrac{1-2\nu}{1-\nu}N_0\Big/N_c}\left(\varepsilon_1 + \frac{\partial^2 \varepsilon_1}{\partial r^2}r_{da}^2\right), \tag{15}$$

where $N_c = \dfrac{k_B T}{K\Delta\Omega_d^2}$.

Substituting (15) into (14), we obtain the deformation equation that, after integration, can be written as

$$\frac{\partial^2 \varepsilon_1}{\partial r^2} - a\varepsilon_1 + f\varepsilon_1^2 - c\varepsilon_1^3 = 0, \tag{16}$$

where $a\left(\varepsilon_0\right) = \dfrac{1 - 2\gamma - 2\delta\gamma^2 - 2|\widetilde{\alpha}|\eta + 3\beta\eta^2}{2r_{da}^2\left(\delta\gamma^2 + \gamma - \dfrac{a_0^2}{2r_{da}^2}\right)}$;

$$f(\varepsilon_0)=\left(|\widetilde{\alpha}|-3\beta\eta\right)\Big/\left(2r_{da}^2\left(\delta\gamma^2+\gamma-\frac{a_0^2}{2r_{da}^2}\right)\right);\quad c=\beta\Big/2\left(r_{da}^2\left(\delta\gamma^2+\gamma-\frac{a_0^2}{2r_{da}^2}\right)\right);\quad \delta=\frac{1}{3}\frac{1-2\nu}{1-\nu};$$

$$\gamma=\frac{N_0/N_c}{1-2\delta N_0/N_c};\quad \eta=\frac{k_BT\gamma}{K\Delta\Omega_d(1+\delta\gamma)}.$$

Here we have taken into account that $\alpha<0,\ \beta>0$.

2. Formation of Nanoclusters and their Periodic Structures

The solution of the equation (16) is

$$r=\int\frac{d\varepsilon_1}{\sqrt{a\varepsilon_1^2-2f\varepsilon_1^3/3+2c\varepsilon_1^4/4}}.$$

Making a substitution $\varepsilon_1=\frac{1}{z}$, one can present this integral as

$$r=-\int dz\Big/\sqrt{a\left(z-\frac{f}{3a}\right)^2+\Delta}, \tag{17}$$

where $\Delta=-\frac{f^2}{9a}+\frac{c}{2}$.

The integral (17) is expressed by the analytic functions whose type we determine by the sign of the coefficients a and Δ.

If the following conditions are fulfilled:

$$0<\gamma<\gamma_c,\ \gamma_c=-\frac{1}{2\delta}+\sqrt{\frac{1}{4\delta^2}+\frac{a_0^2}{2\delta r_{da}^2}}\ \ (a<0 \text{ and } \Delta<0), \tag{18}$$

then $\varepsilon_1=0$, and $N(r)=N_0$, scilicet the distribution of defects is spatially homogeneous.

If parameter γ exceeds the value $\gamma>\gamma_c$, whatever is the supersonic wave deformation amplitude, the spatially nonuniform solution becomes unstable, and there appears a new spatially nonuniform stationary state (formation of clusters or periodic defect structures).

In other cases, depending on the values N_0 and ε_0, the solution of the equation (16) will be:

$$\varepsilon_1(r)=\mathrm{sign}\Delta\Omega_d\frac{A}{B+\mathrm{sh}\left(-\sqrt{a}r\right)},\quad \gamma_c<\gamma<\gamma_{c_1}\quad (a>0 \text{ and } \Delta>0), \tag{19}$$

$$\varepsilon_1(r)=\mathrm{sign}\Delta\Omega_d\frac{A}{B+\mathrm{ch}\left(\sqrt{a}r\right)},\quad \gamma_{c1}<\gamma<\gamma_{c_2}\quad (a>0 \text{ and } \Delta<0), \tag{20}$$

$$\varepsilon_1(r)=\mathrm{sign}\Delta\Omega_d\frac{A}{B+\sin\left(\sqrt{|a|}r\right)},\quad \gamma>\gamma_{c_2}\quad (a<0 \text{ and } \Delta>0), \tag{21}$$

where $\gamma_{c1}(\varepsilon_0)\approx 1/2-\widetilde{\alpha}^2(\varepsilon_0)/9\beta$; $\gamma_{c2}\approx 1/2$; $A=3\sqrt{2}|a|\left(\left|9ca-2f^2\right|\right)^{-\frac{1}{2}}$; $B=fA/3|a|$.

The cluster radius depends on the defect concentration, elastic constants, and can be determined as follows:

$$d(\varepsilon_0)=\frac{1}{\sqrt{a}}=\sqrt{\frac{2r_{da}^2\left(\delta\gamma^2+\gamma-\frac{a_0^2}{2r_{da}^2}\right)}{1-2\gamma-2\delta\gamma^2-2|\tilde{\alpha}|\eta+3\beta\eta^2}}. \quad (22)$$

Ultrasound influences the conditions of formation of the self-organized clusters and their sizes. In general, the cluster size is determined by the characteristic length of interaction between the dot defect and matrix atoms r_{da}, and also parameter γ (the average concentration of defects, the elastic constants of material of semiconductor structure, the temperature and the change in volume of the crystal by one defect $\Delta\Omega_d$). The characteristic length of interaction between the dot defect and matrix atoms r_{da} depends on concentration of defects, i.e. on parameter γ, and can be estimated from the schedule of dependence of the free energy of elastically deformed crystal $\tilde{\Phi}(r_{da})=\int_V \Phi(r,r_{da})dV$ on the r_{da}. As all irreversible processes at a constant temperature are accompanied by decrease in free energy, the placement of impurities in the studied system will meet to such value of r_{da} at which the free energy is minimum.

Fig. 1 shows the dependence of the size of dot defects cluster on value of their relative average concentration without influence of ultrasound (the curve 1) and in case of different values of amplitude of ultrasonic wave (the curves 2, 3 and 4). Calculations were carried out for the GaAs semiconductor with the following parameter values: $T=300°C$; $\Delta\Omega_d=125\ Å^3$; $a_0=5\ Å$; $K=0.45\ eV/Å^3$; $\nu=0.35$; $R_0=0.5\ \mu m$; $\frac{\alpha^2}{\beta}=2$ [17].

As can be seen from fig. 1 without the action of ultrasound the nanocluster size significantly depends on concentration of defects and at change of the relative concentration in range of $0.05\le N_0/N_c\le 0.2$ the nanocluster size increases from 2 *nm* to 6 *nm*.

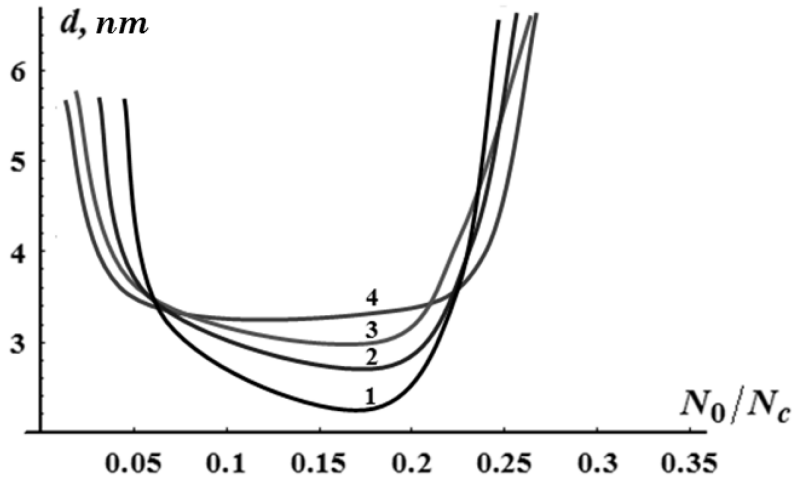

Fig. 1. Dependence of the size of dot defects cluster on value of their relative concentration:
1 – $\varepsilon_0=0$; **2** – $\varepsilon_0=10^{-6}$; **3** – $\varepsilon_0=10^{-5}$; **4** – $\varepsilon_0=5\cdot10^{-5}$

In the presence of ultrasound the change in concentration of defects leads to minor change of the nanocluster size. Thus, at action of ultrasound with amplitude $\varepsilon_0=5\cdot10^{-5}$ (fig. 1, the curve 4) at change of the concentration in the range of $0.05\le N_0/N_c\le 0.2$ the nanocluster radius changes from 3,4 *nm* to 3,6 *nm*. Therefore, we can claim that in the presence of defects with concentration in

the range of $0.05 \le N_0/N_c \le 0.2$ under the action of ultrasound the nanoclusters, uniform in the sizes, will be formed.

The presence of ultrasound leads to a decrease of dispersion of radius of the spherical nanocluster. And increase in amplitude of an ultrasonic wave leads to decrease of dispersion of the nanocluster size. Besides, the ultrasonic treatment expands intervals of the concentration of defects and temperature ranges within which the formation of self-organized nanoclusters is possible.

Thus, treatment by ultrasound of semiconductor materials in the growth process of the self-organized nanoclusters (for example, under the influence of laser irradiation, in the process of the molecular beam epitaxy, etc.) will promote the formation of the nanoclusters, uniform in the sizes. It can be explained by the emergence of additional deformation flux at the expense of the inhomogeneous deformation created by an ultrasonic wave that leads to the restriction of mobility of atoms of the nanocluster [7].

Besides, the presence of ultrasound changes mean value of deformation and, respectively, the value of the surface energy of the array of three-dimensional coherently strained islands (QD). In Ref. [18] it's shown that the character of dependence of the surface energy on the size of islands is defined by the parameter α, which is equal to the relative change of the surface energy at formation of one island. Change of the value of deformation at the expense of ultrasound leads to decrease of parameter α, and, respectively, the system of islands becomes more resistant to coalescence [16].

3. Effect of Ultrasound on the Reducing of Size Dispersion of the of InAs/GaAs Quantum Dots Doped with an Isovalent Impurity

Let a GaAs semiconductor with dot defects of two kinds with the average concentrations N_{d01} (In) and N_{d02} (Bi, P, Sb) undergo the action of an acoustic wave. The non-uniform deformation of this semiconductor material results from two factors: the acoustic wave action and the non-uniform redistribution of dot defects. The expression for the crystal lattice deformation can be presented in the form:

$$\varepsilon(x,t) = \varepsilon_0 \cos\left(\omega t - \frac{\omega}{c_l} x\right) + \frac{\theta_{d1}}{K} N_{d1}(x,t) + \frac{\theta_{d2}}{K} N_{d2}(x,t), \tag{23}$$

where ε_0 is the amplitude of the deformation induced by an acoustic wave with frequency ω; c_l is the longitudinal sound velocity; $\theta_{di} = K\Delta\Omega_i$ is the deformation potential (K is the elasticity modulus, $\Delta\Omega_i$ is the crystal volume change per $i = 1, 2$) defect. For interstitial atoms and substitutional impurities with the ionic radius exceeding the ionic radius of matrix atoms, the deformation potential $\theta_{di} > 0$, whereas, for substitutional impurities with ionic radius smaller than the ionic radius of matrix atoms $\theta_{di} < 0$.

In the linear approximation the system of equations for diffusing defects acquires the form:

$$\frac{\partial N_{di}(x,t)}{\partial t} = D_i \frac{\partial^2 N_{di}(x,t)}{\partial x^2} - \frac{D_i \theta_{di}}{kT} \frac{\partial}{\partial x}\left(N_{di}(x,t) \frac{\partial \varepsilon(x,t)}{\partial x}\right) + G_{di} - \frac{N_{di}(x,t)}{\tau_{di}}. \tag{24}$$

Let us write the defect concentration in the form (11).

Taking Eq. (23) into account and making the approximation $N_d^{(i)} << N_{d0i}$ we obtain the following system of equations for $N_d^i(x,t)$:

$$\frac{\partial N_d^{(1)}(x,t)}{\partial t} = D_1 \frac{\partial^2 N_d^{(1)}(x,t)}{\partial x^2} - D_1 \frac{N_{d01}}{N_{dc1}} \left(\frac{\partial^2 N_d^{(1)}(x,t)}{\partial x^2} + \frac{\theta_{d2}}{\theta_{d1}} \frac{\partial^2 N_d^{(2)}(x,t)}{\partial x^2} - \right.$$

$$\left. - \frac{K}{\theta_{d1}} \varepsilon_0 \left(\frac{\omega}{c_l} \right)^2 \cos\left(\omega t - \frac{\omega}{c_l} x \right) \right) + G'_{d1} - \frac{N_d^{(1)}(x,t)}{\tau_{d1}}, \quad (25)$$

$$\frac{\partial N_d^{(2)}(x,t)}{\partial t} = D_2 \frac{\partial^2 N_d^{(2)}(x,t)}{\partial x^2} - D_2 \frac{N_{d02}}{N_{dc2}} \left(\frac{\partial^2 N_d^{(2)}(x,t)}{\partial x^2} + \frac{\theta_{d1}}{\theta_{d2}} \frac{\partial^2 N_d^{(1)}(x,t)}{\partial x^2} - \right.$$

$$\left. - \frac{K}{\theta_{d2}} \varepsilon_0 \left(\frac{\omega}{c_l} \right)^2 \cos\left(\omega t - \frac{\omega}{c_l} x \right) \right) + G'_{d2} - \frac{N_d^{(2)}(x,t)}{\tau_{d2}}, \quad (26)$$

where $N_{dci} = \frac{K \cdot kT}{\theta_{di}^2}$; $G'_{di} = G_{di} - \frac{N_{d0i}}{\tau_{di}}$.

In order to find a solution of the system of differential equations (25) and (26), let us apply the integral Laplace transformation:

$$X_i(x,p) = \int_0^\infty N_d^{(i)}(x,t) e^{-pt} dt. \quad (27)$$

Then the system of equations (25) and (26) reads:

$$pX_1 - N_d^{(1)}(x,0) = D_1 \left(1 - \frac{N_{d01}}{N_{dc1}} \right) \frac{\partial^2 X_1}{\partial x^2} + \frac{G'_{d1}}{p} - \frac{X_1}{\tau_{d1}} - D_1 \frac{N_{d01}}{N_{dc1}} \frac{\theta_{d2}}{\theta_{d1}} \frac{\partial^2 X_2}{\partial x^2} +$$

$$+ D_1 \frac{N_{d01}}{N_{dc1}} \frac{K}{\theta_{d1}} \varepsilon_0 \left(\frac{\omega}{c_l} \right)^2 \left(\frac{p}{p^2 + \omega^2} \cos\left(\frac{\omega}{c_l} x \right) + \frac{\omega}{p^2 + \omega^2} \sin\left(\frac{\omega}{c_l} x \right) \right), \quad (28)$$

$$pX_2 - N_d^{(2)}(x,0) = D_2 \left(1 - \frac{N_{d02}}{N_{dc2}} \right) \frac{\partial^2 X_2}{\partial x^2} + \frac{G'_{d2}}{p} - \frac{X_2}{\tau_{d2}} - D_2 \frac{N_{d02}}{N_{dc2}} \frac{\theta_{d1}}{\theta_{d2}} \frac{\partial^2 X_1}{\partial x^2} +$$

$$+ D_2 \frac{N_{d02}}{N_{dc2}} \frac{K}{\theta_{d2}} \varepsilon_0 \left(\frac{\omega}{c_l} \right)^2 \left(\frac{p}{p^2 + \omega^2} \cos\left(\frac{\omega}{c_l} x \right) + \frac{\omega}{p^2 + \omega^2} \sin\left(\frac{\omega}{c_l} x \right) \right), \quad (29)$$

where $N_d^{(i)}(x,0)$ is the spatially non-uniform component of the initial distribution of defect concentration.

By finding the solution of the system of differential equations (28) and (29), which is finite as $x \to \pm\infty$ and satisfies the initial condition $N_d^{(i)}(x,0) = 0$, and applying the inverse Laplace transformation, we obtain the space-time redistribution of dot defects of both kinds, $N_{d1}(x,t)$ and $N_{d2}(x,t)$, under the influence of an acoustic wave and the strain distribution $\varepsilon(x,t)$ created by both ultrasound and dot defects.

On the basis of the developed model, let us analyze the possibility to reduce the size dispersion of strained InAs/GaAs QDs doped with an isovalent impurity with the help of ultrasound. Let us consider a semiconductor structure with an InAs/GaAs QD doped with an isovalent impurity. The

latter is an As-atom substitutional defect. Depending on impurity's ionic radius r_i, the increase of the QD volume amounts to $\Delta\Omega_i = \frac{4}{3}\pi(r_i^3 - r_{\text{As}}^3)$.

Numerical calculations were carried out for the following parameters: $\omega = 10^{11}\ s^{-1}$; $\varepsilon_0 = 0{,}00001$; $\tau_{di} = 0{,}001\ ms$; $K = 6500\ eV/nm^3$; $c_l = 3500\ m/s$; $r_i(\text{Ga}^{3+}) = 0{,}062\ nm$; $r_i(\text{In}^{3+}) = 0{,}092\ nm$; $r_i(\text{As}^{3+}) = 0{,}069\ nm$; $r_i(\text{Bi}^{3+}) = 0{,}12\ nm$; $r_i(\text{Sb}^{3+}) = 0{,}082\ nm$; $r_i(\text{P}^{3+}) = 0{,}044\ nm$; $D_{\text{In}} = 6\cdot 10^5 \exp\left(-\frac{4}{kT}\right) cm^2/s$;[6] $D_{\text{P}} = 1{,}26\cdot 10^2 \exp\left(-\frac{2{,}7}{kT}\right) cm^2/s$.[19] There are no data in the scientific literature concerning the temperature dependences of the diffusion coefficients for Bi and Sb in InAs. Therefore, in calculations, we used the same values as for P.

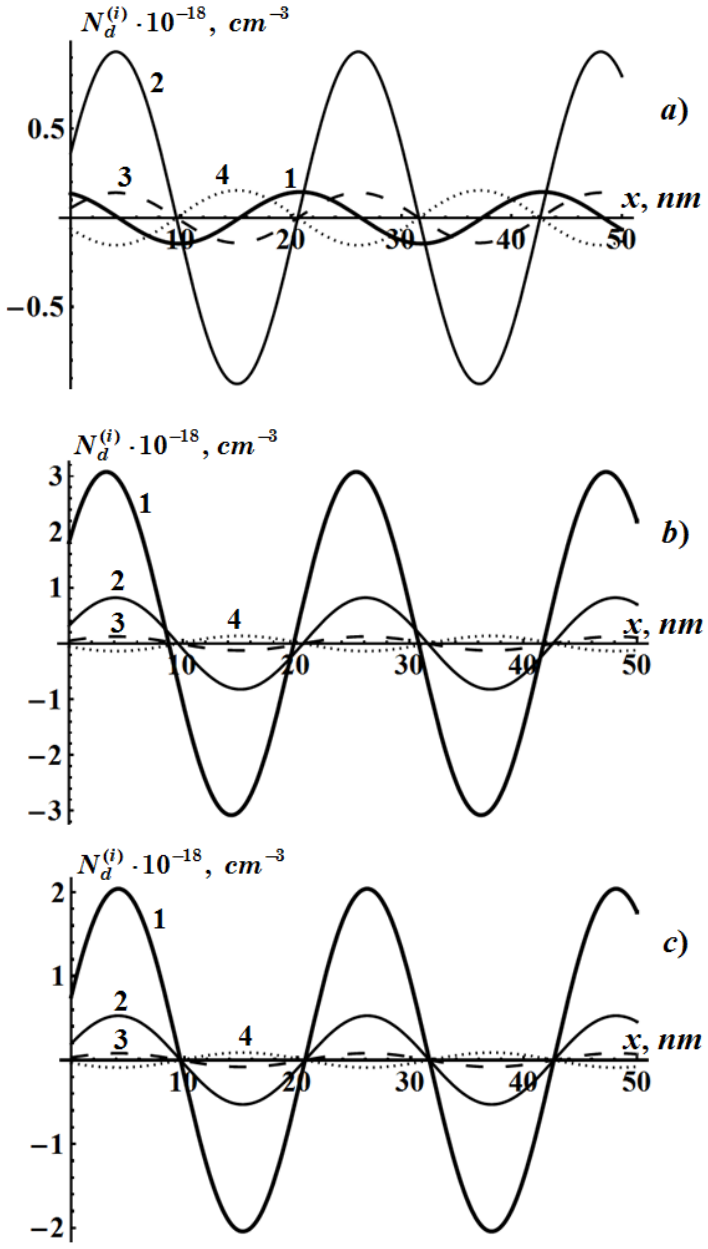

Fig. 2. Spatial redistributions of In (**1**), Bi (**2**), Sb (**3**) and P (**4**) at various temperatures $T = 450\ K$ (*a*), $T = 600\ K$ (*b*), $T = 900\ K$ (*c*)

In Fig. 2, the spatial redistributions of In, which is a substitutional defect, with the concentration ($N_{d0\text{In}} = 10^{20}\ cm^{-3}$) (curve 1) and the isovalent impurities Bi, Sb, and P (curves 2, 3, and 4,

respectively) in the GaAs matrix under the action of an acoustic wave at various temperatures are shown. In the temperature interval 600 – 900 *K* (Figs. 2, b and c), the ultrasonic wave favors the accumulation of In and Bi (Sb) in the same spatial regions. This fact should promote the size uniformity enhancement over the QD array. The strain gradient is much larger if Bi impurities are available, which is associated with a larger difference between the ionic radii of Bi^{3+} and As^{3+} in comparison with that between Sb^{3+} and As^{3+}. On the contrary, In and P are accumulated in different spatial regions, which should result in a larger dispersion of the QD sizes. This conclusion follows from the fact that the ionic radius of P^{3+} is smaller than that of As^{3+}, so that the P impurities are localized at the strain minima.

However, by lowering the temperature ($T < 500$ *K*), it is possible to obtain a partial overlapping of the regions, where the P and In impurities are accumulated (Fig. 2, a). In this case, on the contrary, a delocalization of In atoms around the Sb and Bi impurities is observed. The largest shift of the In concentration maximum with respect to impurities amounts to a quarter-wavelength.

The obtained results qualitatively agree with the experimental data of Ref. [11]. Namely, it was found that the ultrasonic treatment of semiconductor quantum dots for 5 – 90 *min* in the course of their synthesis allows one to obtain nanoclusters that are more uniform by dimensions.

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