SELF-ORGANIZED DIFFUSION-DEFORMATION DISTRIBUTION OF POINT DEFECTS IN STRESSED HETEROSYSTEMS

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A nonlinear model of the self-organized redistribution of point defects in three-layer GaAs/InAs/GaAs and ZnTe/CdTe/ZnTe heterosystems has been developed. It has been demonstrated that the concentration profile of point defects can vary substantially depending on their average concentration and the width of the internal stressed layer.

1. Introduction

By means of external factors, such as laser or particle irradiation, one can create point defects – interstitial atoms and vacancies – and control their number in the crystal by changing the intensity of irradiation [1, 2]. The self-organization of induced defects, which interact with one another through the field of elastic continuum deformations, was studied earlier in isotropic solids [2–4]. In particular, in work [2], a theory was developed for the formation of a hierarchy of stationary one-dimensional defect-deformational (DD) structures in irradiated crystals. It has been demonstrated that, depending on the level of the excess of the spatially homogeneous concentration of defects N_{d0} over the corresponding threshold values, stationary localized DD-mesostructures are formed first, followed by the formation of periodic mesostructures.

Recently, GaAs/InAs/GaAs and ZnTe/CdTe/ZnTe heterostructures with stressed quantum wells have been widely used in microelectronic devices. To ensure the operational reliability of such devices and to create the devices with prescribed physical properties, the study of the mechanism of defect distribution in such crystalline systems is of importance. In this work, a model for the phenomenon of point defect self-organization in three-layer stressed heterostructures – in particular, GaAs/InAs/GaAs and ZnTe/CdTe/ZnTe ones – has been developed.

2. Model

Consider stressed heterosystems (GaAs/InAs/GaAs or ZnTe/CdTe/ZnTe ones) with an interlayer (InAs or CdTe, respectively) of the thickness $2a$ (Fig. 1). Suppose that the external GaAs (ZnTe) layers do not undergo a deformation, because their thickness considerably exceeds the width of the interlayer. The mechanical deformation, which arises owing to a mismatch between the lattice parameters of the contacting materials, is approximated by the function

$$\varepsilon^{(i)}(x) = \begin{cases} \varepsilon_0 \dfrac{x^2}{a^2}, & i = 2; \\ 0, & i = 1, 3; \end{cases} \tag{1}$$

where $\varepsilon_0 = \varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz} < 0$; $\varepsilon_{yy} = \varepsilon_{zz} = (a_s - a_0)/a_s$; $\varepsilon_{xx} = -2\left(C_{12}^{(2)}/C_{11}^{(2)}\right)\varepsilon_{yy}$; the superscripts $i = 1$ and 3 correspond to the GaAs (ZnTe) layers and the superscript $i = 2$ to the InAs (CdTe) interlayer; a_s and a_0 are the lattice parameters of GaAs (ZnTe) and InAs (CdTe), respectively; and $C_{11}^{(2)}$ and $C_{12}^{(2)}$ are the elastic constants of InAs (CdTe).

Let point defects be distributed in this crystal system with the average concentration N_{d0}. To find the spatial redistribution of point defects, one has to solve the system of coupled equations for the medium deformation $U(x)$ and the defect concentration $N_d(x)$. The stationary

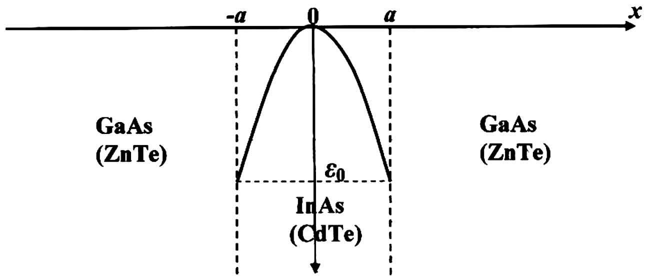

Fig. 1. Scheme of GaAs/InAs/GaAs and ZnTe/CdTe/ZnTe heterostructures with stressed layers (InAs or CdTe, respectively)

equation of diffusion looks like

$$D_d^{(i)}\frac{\partial^2 N_d^{(i)}}{\partial x^2}-\frac{D_d^{(i)}\theta_d^{(i)}}{kT}\times$$

$$\times\frac{\partial}{\partial x}\left(N_d^{(i)}\left(\frac{\partial U^{(i)}}{\partial x}+\left(l_d^{(i)}\right)^2\frac{\partial^3 U^{(i)}}{\partial x^3}\right)\right)=0, \quad (2)$$

where D_d is the diffusion coefficient of point defects, $\theta_d = K_A\Delta\Omega$ is the deformation potential, K_A the elastic constant of uniform compression, $\Delta\Omega$ the variation of the crystal volume caused by the formation of one defect, and $l_d^{(i)}$ the characteristic length of the interaction between defects and crystal atoms.

The equation, which describes a deformation in the heterosystem taking into account the deformation caused by a mismatch between the lattice parameters of contacting materials, has the form [2]

$$\frac{\partial^2 U^{(i)}(x)}{\partial x^2}+\left(l_0^{(i)}\right)^2\frac{\partial^4 U^{(i)}(x)}{\partial x^4}-$$

$$-\left|\alpha^{(i)}\right|\frac{\partial^2\left(\left(U^{(i)}(x)\right)^2\right)}{\partial x^2}+\beta^{(i)}\frac{\partial^2\left(\left(U^{(i)}(x)\right)^3\right)}{\partial x^2}-$$

$$-\frac{\theta_d^{(i)}}{\rho^{(i)}\left(c_l^{(i)}\right)^2}\frac{\partial^2 N_d^{(i)}(x)}{\partial x^2}-\frac{\partial^2\varepsilon^{(i)}(x)}{\partial x^2}=0, \quad (3)$$

where $\rho^{(i)}$ are the densities of materials composing the heterosystem, $c_l^{(i)}$ the longitudinal speed of sound, $l_0^{(i)}$ the characteristic length of the interatomic interaction, and $\alpha^{(i)}$ and $\beta^{(i)}$ are the constants of elastic anharmonicity.

The solutions of the differential equations (2) and (3) are searched in each region of the heterosystem with point defects. The following conditions must be satisfied at the layer interfaces:

$$N^{(i)}(\pm\infty)=N_{d0},\quad J^{(1)}(-a)=J^{(2)}(-a),$$

$$J^{(i)}(\pm\infty)=0;\quad J^{(3)}(a)=J^{(2)}(a),$$

$$N^{(1)}(-a)=N^{(2)}(-a),\quad \sigma_{xx}^{(1)}(-a)=\sigma_{xx}^{(2)}(-a),$$

$$N^{(3)}(a)=N^{(2)}(a),\quad \sigma_{xx}^{(3)}(a)=\sigma_{xx}^{(2)}(a). \quad (4)$$

Here,

$$J^{(i)}(x)=-D_d^{(i)}\frac{\partial N_d^{(i)}}{\partial x}+\frac{D_d^{(i)}\theta_d^{(i)}}{kT}N_d^{(i)}\times$$

$$\times\left(\frac{\partial U^{(i)}}{\partial x}+\left(l_d^{(i)}\right)^2\frac{\partial^3 U^{(i)}}{\partial x^3}\right)$$

is the total flux of defects (the first term corresponds to the usual diffusive flux of defects; the second term describes the interaction between point defects and the elastic medium);

$$\sigma_{xx}^{(i)}=\frac{E_i}{(1+\nu_i)(1-2\nu_i)}\left[(1+\nu_i)U_{xx}^{(i)}+\nu_i\left(U_{yy}^{(i)}+U_{zz}^{(i)}\right)\right]$$

is the normal component of the mechanical stress; E_i, ν_i is Young's modulus of materials of the heterosystem, ν_i are their Poisson's ratios; and $U_{xx}^{(i)}$, $U_{yy}^{(i)}$, and $U_{zz}^{(i)}$ are the components of the deformation tensor. Let the number of defects in the heterostructure remain constant, i.e. let the condition

$$\int_{-\infty}^{\infty}(N_d(x)-N_{d0})dx=0. \quad (5)$$

be satisfied.

The deformation and the defect concentration can be written in the form

$$U(x)=U_0+U_l(x),\quad N_d(x)=N_{d0}+N_{dl}(x), \quad (6)$$

where $U_l(x)$ and $N_{dl}(x)$ are the spatially inhomogeneous components of the deformation and the defect concentration, respectively; and $U_0^{(i)}=\frac{\theta_d^{(i)}}{K_A^{(i)}}N_{d0}$ is the spatially averaged deformation.

While solving Eq. (2) in the approximation

$$\frac{\theta_d^{(i)}}{kT}\left(U_l^{(i)}+\left(l_d^{(i)}\right)^2\frac{\partial^2 U_l^{(i)}}{\partial x^2}\right)\ll 1$$

and taking Eq. (6) into account, we obtain the following expression for the spatially inhomogeneous concentration of defects:

$$N_{dl}^{(i)}(x)=\begin{cases}\frac{\theta_d^{(i)}N_{d0}}{kT}\left(U_l^{(i)}+\left(l_d^{(i)}\right)^2\frac{\partial^2 U_l^{(i)}}{\partial x^2}\right),\ i=1,3;\\ \frac{\theta_d^{(i)}N_{d0}}{kT}\left(U_l^{(i)}+\left(l_d^{(i)}\right)^2\frac{\partial^2 U_l^{(i)}}{\partial x^2}\right)+N^*,\ i=2,\end{cases}\tag{7}$$

where N^* is a constant of integration. Substituting Eq. (7) into Eq. (3), we obtain the equation for the spatially inhomogeneous component of medium deformation

$$\frac{\partial^2 U^{(i)}(x)}{\partial x^2}+\left(l_d^{(i)}\right)^2\frac{\partial^4 U^{(i)}(x)}{\partial x^4}-$$
$$-\left|\alpha^{(i)}\right|\frac{\partial^2\left(\left(U^{(i)}(x)\right)^2\right)}{\partial x^2}+\beta^{(i)}\frac{\partial^2\left(\left(U^{(i)}(x)\right)^3\right)}{\partial x^2}-$$
$$-\frac{\left(\theta_d^{(i)}\right)^2 N_{d0}}{\rho^{(i)}\left(c_l^{(i)}\right)^2 kT}\left(\frac{\partial^2 U_l^{(i)}}{\partial x^2}+\left(l_d^{(i)}\right)^2\frac{\partial^4 U_l^{(i)}}{\partial x^4}\right)-$$
$$-\frac{\partial^2\varepsilon^{(i)}(x)}{\partial x^2}=0.\tag{8}$$

Integrating this equation, we obtain

$$\frac{\partial^2 U_l^{(i)}}{\partial x^2}-a^{(i)}U_l^{(i)}+f^{(i)}\left(U_l^{(i)}\right)^2-c^{(i)}\left(U_l^{(i)}\right)^3=$$
$$=-\frac{\varepsilon^{(i)}(x)}{\left(l_d^{(i)}\right)^2\frac{N_{d0}}{N_{dc}^{(i)}}-\left(l_0^{(i)}\right)^2}+b_1^{(i)}x+b_0^{(i)},\tag{9}$$

where

$$a^{(i)}=\frac{1-N_{d0}/N_{dc}^{(i)}}{l_d^2N_{d0}/N_{dc}^{(i)}-l_0^{(i)2}},\quad f=\frac{\left|\alpha^{(i)}\right|}{l_d^2N_{d0}/N_{dc}^{(i)}-l_0^{(i)2}},$$

$$c=\frac{\left|\beta^{(i)}\right|}{l_d^2\frac{N_{d0}}{N_{dc}^{(i)}}-l_0^{(i)2}},$$

and

$$N_{dc}^{(i)}=\frac{\rho^{(i)}\left(c_l^{(i)}\right)^2 kT}{\left(\theta_d^{(i)}\right)^2}$$

is the critical concentration of defects.

For the condition $U_l(\pm\infty)=0$ to be satisfied, the equalities $b_1^{(i)}=0$ and $b_0^{(i)}=0$ for $i=1$ and 3 must hold true.

The solution of Eq. (9) is tried in the form $U_l^{(i)}(x)=U_{0l}^{(i)}(x)+U_{1l}^{(i)}(x)$, where $U_{0l}^{(i)}(x)$ is the solution of the corresponding homogeneous equation. For $i=1$ and 3, the relation $U_l^{(i)}(x)=U_{0l}^{(i)}(x)$ is valid. Depending on the average concentration of point defects N_{d0}, the dependence $U_{0l}^{(i)}(x)$ looks like [2]

$$U_{0l}^{(i)}(x)=\ 0,\quad N_{d0}<N_{dc1}^{(i)},\tag{10}$$

$$U_{0l}^{(i)}(x)=\ \mathrm{sign}\theta_d^{(i)}\frac{A^{(i)}}{B^{(i)}+\mathrm{sh}(-\sqrt{a^{(i)}}x)},\quad N_{dc1}^{(i)}<N_{d0}<N_{dc2}^{(i)},\tag{11}$$

$$U_{0l}^{(i)}(x)=\mathrm{sign}\theta_d^{(i)}\frac{A^{(i)}}{B^{(i)}+\mathrm{ch}(\sqrt{a^{(i)}}x)},\quad N_{dc2}^{(i)}<N_{d0}<N_{dc}^{(i)},\tag{12}$$

$$U_{0l}^{(i)}(x)=\mathrm{sign}\theta_d^{(i)}\frac{A^{(i)}}{B^{(i)}+\sin(\sqrt{\left|a^{(i)}\right|}x)},\quad N_{d0}>N_{dc}^{(i)},\tag{13}$$

where

$$A^{(i)}=3\sqrt{2}\left|a^{(i)}\right|\left(\left|9c^{(i)}a^{(i)}-2f^{(i)2}\right|\right)^{-1/2},$$
$$B^{(i)}=\sqrt{2}f^{(i)}\left(\left|9c^{(i)}a^{(i)}-2f^{(i)2}\right|\right)^{-1/2},$$

$N_{dc1}^{(i)}=N_{dc}^{(i)}\left(l_0^{(i)}/l_d^{(i)}\right)^2$, $N_{dc2}^{(i)}=N_{dc}^{(i)}\left\{1-\frac{2[\alpha^{(i)}]^2}{9\beta^{(i)}}\right\}$, and $\frac{2[\alpha^{(i)}]^2}{9\beta^{(i)}}=\frac{4}{9}$.

The deformation $U_{1l}^{(2)}(x)$ is determined from the equation

$$\frac{\partial^2 U_{1l}^{(2)}}{\partial x^2}-a^{(2)}U_{1l}^{(2)}+f^{(2)}\left(U_{1l}^{(2)}\right)^2+2f^{(2)}U_{0l}^{(2)}U_{1l}^{(2)}-$$
$$-c^{(2)}\left(U_{1l}{}^{(2)}\right)^3-3c^{(2)}\left(U_{0l}^{(2)}\right)^2U_{1l}^{(2)}-3c^{(2)}U_{0l}^{(2)}\left(U_{1l}^{(2)}\right)^2=$$
$$=-\frac{\varepsilon^{(2)}(x)}{\left(l_d^{(2)}\right)^2\frac{N_{d0}}{N_{dc}^{(2)}}-\left(l_0^{(2)}\right)^2}+b_1^{(2)}x+b_0^{(2)}.\tag{14}$$

Since the deformation parameter $U_{1l}^{(2)}(x)<1$, the estimation of the solution can be done if one neglects

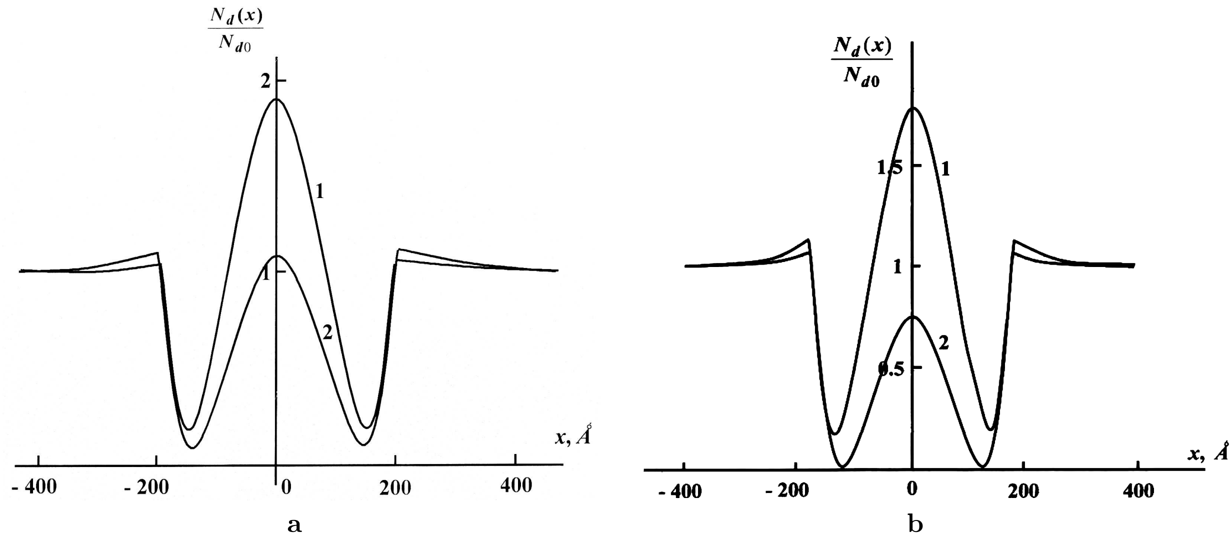

Fig. 2. Redistribution of point defects in a GaAs/InAs/GaAs heterostructure for various widths of the stressed InAs interlayer $2a = 400$ (panel *a*) and 360 Å (panel *b*), and various average defect concentrations $N_{d0}/N_{dc} = 0.59$ (curves *1*) and 0.79 (curves *2*)

quadratic and cubic terms. In this case, $U_{1l}^{(2)}(x)$ looks like

$$U_{1l}^{(2)}(x) = C_1 e^{-\sqrt{a^{(2)}}x} + C_2 e^{\sqrt{a^{(2)}}x} + \frac{\varepsilon_0 \frac{x^2}{a^2}}{1 - \frac{N_{d0}}{N_{dc}{}^{(2)}}} + b_1 x + b_0, \quad (15)$$

where b_1 and b_0 are some constants.

3. Calculation Results and Their Discussion

In the case $N_{d0} < N_{dc1}$, there is no process of defect self-organization, and the results of this work are in qualitative agreement with those obtained in work [5]. In this case, interstitial atoms are accumulated in the stressed InAs or CdTe layer, and the concentration of vacancies becomes reduced in comparison with its average value.

Consider the case where the average concentration of point defects falls within the range $N_{dc2} < N_{d0} < N_{dc}$. In this case, the total deformation and the spatial distribution of point defects look like

$$U^{(i)}(x) = U_0^{(i)} + \operatorname{sign}\theta_d^{(i)} \frac{A^{(i)}}{B^{(i)} + \operatorname{ch}\left(\sqrt{a^{(i)}}x\right)} +$$

$$+\begin{cases} C_1 e^{-\sqrt{a^{(2)}}x} + C_2 e^{\sqrt{a^{(2)}}x} + \dfrac{\varepsilon_0 \frac{x^2}{a^2}}{1 - \frac{N_{d0}}{N_{dc}^{(2)}}} + \\ +b_1 x + b_0, \quad i = 2; \\ 0, \quad i = 1, 3; \end{cases} \quad (16)$$

$$N_d^{(i)}(x) = N_{d0} + \frac{\theta_d^{(i)} N_{d0}}{kT} N_{dl}^{(i)} \left(U_l^{(i)} + \left(l_d^{(i)}\right)^2 \frac{\partial^2 U_l^{(i)}}{\partial x^2} \right) +$$

$$+\begin{cases} 0, & i = 1, 3; \\ N^*, & i = 2. \end{cases} \quad (17)$$

The constants of integration N^*, C_1, C_2, b_0, and b_1 are determined from the boundary conditions (4) and (5). The results of calculations of the deformation parameter $U(x)$ and the concentration of point defects $N_d(x)$ are presented in Figs. 2 and 3. Calculations were carried out for a GaAs/InAs/GaAs heterostructure with the following parameters [2, 6]: $a_s = 5.65$ Å, $a_0 = 6.08$ Å, $C_{11}^{(2)} = 0.833$ Mbar, $C_{12}^{(2)} = 0.453$ Mbar, $C_{11}^{(1)} = 1.223$ Mbar, $C_{12}^{(1)} = 0.571$ Mbar, $l_d^{(i)} = 29$ Å, $l_0^{(i)} = 5$ Å, $T = 300$ K, $\theta_d^{(i)} = 1$ eV, $\rho^{(2)}\left(c_l^{(2)}\right)^2 = 0.58$ Mbar, and $\rho^{(1)}\left(c_l^{(1)}\right)^2 = 0.79$ Mbar.

As a rule, point defects are generated in pairs "interstitial atom – vacancy". But the deformation potential θ_d for interstitial atoms is much higher than that for vacancies. Therefore, one may retain only the term associated with interstitial point defects both in the equation for a deformation and the diffusion equation.

In Figs. 2,*a* and 3,*a*, the distributions of point defects and the coordinate dependences of deformation parameter in a heterostructure with the width of the stressed InAs interlayer $2a = 400$ Å are depicted. In the

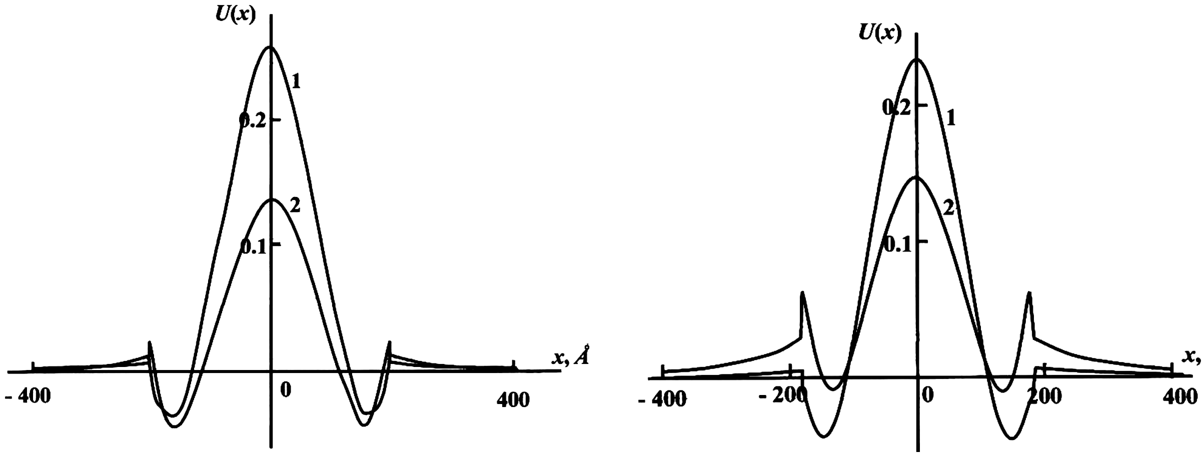

Fig. 3. Coordinate dependences of the deformation parameter in a GaAs/InAs/GaAs heterostructure for various widths of the stressed InAs interlayer $2a = 400$ (panel *a*) and 360 Å (panel *b*), and various average defect concentrations $N_{d0}/N_{dc} = 0.59$ (curves *1*) and 0.79 (curves *2*)

middle of the heterostructure, an excess of the point defect concentration over its average value N_{d0} is observed, while the number of defects decreases near the boundaries of the stressed interlayer. In whole, the number of defects in the stressed InAs interlayer diminishes by 10–50% in comparison with its average value. The character of the point defect distribution in heterostructures is governed by the deformation one. Lattice deformation is caused by two self-consistent factors: (i) a mismatch between the lattice parameters of contacting materials and (ii) the spatial redistribution of point defects. The former factor dominates near the heterostructure's interfaces (Fig. 3,*a*); hence, the crystal lattice undergoes a squeezing deformation. At some distance from the heterointerface, the deformation component associated with the mismatch between the lattice parameters decreases; and the character of the lattice deformation is determined by the redistribution of point defects.

As the width of the stressed InAs interlayer decreases down to 360 Å (Fig. 3,*b*), the number of point defects ($\theta_d > 0$) in it becomes reduced by 15-80% with respect to the average value. In experimental works [7, 8], the intensity of photoluminescence in heterosystems with stressed quantum wells was shown to be lower than that in heterosystems with no stressed layers. It can be explained by the reduction of the defect number in the working region.

The difference between the reduced number of point defects in the stressed layer and the defect number obtained in the case of their spatially homogeneous distribution depends on both the interlayer width and the average defect concentration (Figs. 2,*a* and 2,*b*). In particular, the number of point defects in the stressed InAs interlayer diminishes as their average concentration increases.

In the heterostructure with a stressed interlayer, which undergoes a tensile deformation, the number of defects remains practically unchanged in comparison that in the case of their spatially homogeneous distribution.

If the critical concentration N_{cd} becomes exceeded, the interaction between the system of point defects and the elastic medium gives rise to the formation of periodic deformation structures.

4. Conclusions

1. The phenomenon of point defect self-organization in stressed heterosystems was demonstrated to give rise to a reduction of the average concentration of point defects in the stressed squeezed interlayer in comparison with that under their spatially homogeneous distribution: by 10% at $a = 200$ Å and $N_{d0}/N_{dc} = 0.59$, and by 70% at $a = 180$ Å and $N_{d0}/N_{dc} = 0.79$.
2. Self-organization effects were established to give rise to the emergence of a nonmonotonous dependence of the concentration profile of point defects in the vicinity of heterointerfaces. The structure of the stressed interlayer near a heterointerface becomes more perfect as compared with that of external layers.

3. Self-organization effects were established to give rise to the emergence of a nonmonotonous coordinate dependence of the crystal lattice deformation parameter in the interlayer near the heterointerfaces. If the spatially homogeneous concentration of defects is sufficiently high, $N_{d0} < N_{dc1}$, the nonmonotonous character of this deformation disappears.

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САМООРГАНІЗОВАНИЙ ДИФУЗІЙНО-ДЕФОРМАЦІЙНИЙ РОЗПОДІЛ ТОЧКОВИХ ДЕФЕКТІВ У НАПРУЖЕНИХ ГЕТЕРОСИСТЕМАХ

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Р е з ю м е

Побудовано нелінійну модель самоорганізованого перерозподілу точкових дефектів в тришарових гетеросистемах GaAs/InAs/GaAs, ZnTe/CdTe/ZnTe. Показано, що в залежності від ширини внутрішнього напруженого шару та середньої концентрації точкових дефектів їх концентраційний профіль може суттєво змінюватися.