LATTICE DEFORMATION AND THE SPATIAL REDISTRIBUTION OF POINT DEFECTS IN A STRESSED EPITAXIAL LAYER

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A model of the deformation-diffusion phenomena in stressed epitaxial layers has been constructed on the basis of the self-consistent system of equations for the defect concentration and the deformation parameter. The calculations of the stationary profile of point defects (interstitial atoms and vacancies) and the lattice deformation parameter in InAs epitaxial layers grown on the GaAs substrate have been carried out. The dependence of the deformation parameter on the distance from the heterointerface has been shown nonmonotonous provided that there are point defects in the epitaxial layer.

1. Introduction

The optical and electric properties of semiconductor devices, which are based on quantum wells, are known to depend significantly on both the lattice deformation and the spatial distribution of point defects in the epitaxial layer [1]. The interaction between defects and the self-consisted field of deformation results in the formation of ordered defect-deformational (DD) structures, in particular, clusters and periodic structures [2].

A new aspect of the theory of self-organization of DD structures has been considered in work [3]. In particular, it has been shown that provided a rather high concentration of point defects, the character of the deformation field created by a point defect in an isotropic solid changes.

In this work, the lattice deformation and the redistribution of point defects are investigated on the basis of the self-consistent system of equations for the deformation of and the defect concentration in a stressed epitaxial layer.

2. Model

Let point defects be distributed with the average concentration n_{d0} in a stressed epitaxial layer grown on a thick substrate ($h_s \gg h_0$, where h_s and h_0 are the thicknesses of the substrate and the grown layer, respectively). Owing to a mismatch between the lattice parameters of the substrate and the grown layer, there appears a deformation $\xi\left(x\right)$ in the latter. On moving away from the heterointerface towards the axis of growth, the lattice deformation is modeled by the exponential function

$$\xi(x)=\xi_0 e^{-\alpha x}, x\geq 0, \tag{1}$$

where

$$\xi_0=\xi_{xx}+\xi_{yy}+\xi_{zz},\quad \xi_{yy}=\xi_{zz}=\frac{a_s-a_0}{a_s},$$

$$\xi_{xx}=-\frac{2C_{12}}{C_{11}}\xi_{yy}, \tag{2}$$

is the relative change of the elementary cell volume in the grown layer at the heterointerface,

$$\xi_{yy}=\xi_{zz}=\frac{a_s-a_0}{a_s},\quad \xi_{xx}=-\frac{2C_{12}}{C_{11}}\xi_{yy},$$

are the components of the deformation tensor; a_s and a_0 the lattice parameters of the substrate and the epitaxial layer, respectively; C_{11} and C_{12} are the elastic constants; and α is the quantity that is reciprocal to the effective screening radius of the deformation field and depends on the elastic constants.

Such a deformation $\xi(x)$ is renormalized self-consistently by a spatial redistribution of mobile point defects possessing the concentration $n_d(x)$.

The equation for the renormalized deformation $\varepsilon(x)$ looks like [3]

$$\frac{1}{c_l^2}\frac{\partial^2\varepsilon}{\partial t^2}=\frac{\partial^2\varepsilon(x)}{\partial x^2}-\frac{\theta_d}{\rho c_l^2}\frac{\partial^2 n_d(x)}{\partial x^2}-\alpha^2\xi_0 e^{-\alpha x}, \tag{3}$$

where $\theta_d = K\Delta\Omega$ is the deformation potential, K the elastic modulus, $\Delta\Omega$ the variation of the crystal volume after a single defect having been created, c_l the longitudinal speed of sound, and ρ the density of the material of the grown layer.

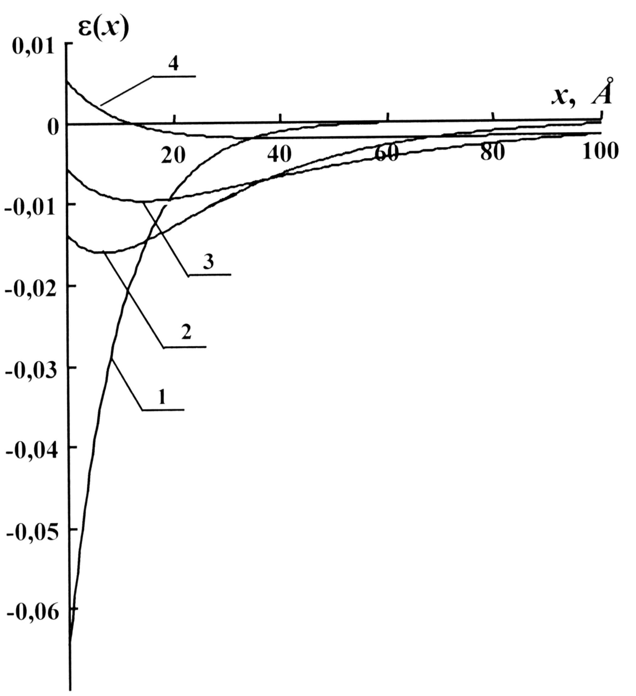


Fig. 1. Coordinate dependences of the deformation parameter of the epitaxial layer for various average values of the point defect concentration $n_{d0} = 0$ (*1*), $0.4n_{dc}$ (*2*), $0.7n_{dc}$ (*3*), and $0.99n_{dc}$ (*4*)

The equation for the defect concentration has the form [2]

$$\frac{\partial n_d(x)}{\partial t} = D\frac{\partial^2 n_d(x)}{\partial x^2} - D\frac{\theta_d}{kT}\frac{\partial}{\partial x}\times$$

$$\times\left[n_d(x)\left(\frac{\partial\varepsilon(x)}{\partial x} + l_d^2\frac{\partial^3\varepsilon(x)}{\partial x^3}\right)\right] + G_d - \frac{n_d(x)}{\tau_d}, \qquad (4)$$

where D is the diffusion coefficient of point defects, l_d the interaction length between the defects and the crystal atoms, G_d the generation rate of point defects by an external source, and τ_d the lifetime of defects.

Below, we consider the stationary state of the DD system, i.e. supposing the conditions $\frac{\partial n_d(x)}{\partial t} = 0$ and $\frac{\partial\varepsilon(x)}{\partial t} = 0$.

Neglecting the defect recombination ($\tau_d^{-1} = 0$), the solution of Eq. (4) reads

$$n_d(x) = n_{d_0}\exp\left(\frac{\theta_d}{kT}\left(\varepsilon(x) + l_d^2\frac{\partial^2\varepsilon(x)}{\partial x^2}\right)\right) \approx$$

$$\approx n_{d_0}\left(1 + \frac{\theta_d}{kT}\left(\varepsilon(x) + l_d^2\frac{\partial^2\varepsilon(x)}{\partial x^2}\right)\right). \qquad (5)$$

The last approximate equality takes place provided that $\frac{\theta_d}{kT}\left(\varepsilon(x) + l_d^2\frac{\partial^2\varepsilon(x)}{\partial x^2}\right) \ll 1$.

Substituting Eq. (5) into Eq. (3), we obtain

$$\frac{\partial^2\varepsilon(x)}{\partial x^2} - \frac{1}{d^2}\varepsilon(x) = -\frac{n_{dc}}{n_{d0}}\frac{1}{l_d^2}\xi_0 e^{-\alpha x}, \qquad (6)$$

where $d^2 = l_d^2\frac{n_{d0}}{n_{dc}}\left(1 - \frac{n_{d0}}{n_{dc}}\right)^{-1}$ and $n_{dc} = \frac{\rho c_l^2 kT}{\theta_d^2}$.

Provided the extra condition

$$\int\limits_0^\infty (n_d(x) - n_{d0})\,dx = 0, \qquad (7)$$

the solution of Eq. (6) at $n_{d0} < n_{dc}$ looks like

$$\varepsilon(x) = \frac{n_{dc}}{n_{d0}}\frac{\xi_0}{l_d^2}\frac{1}{\frac{1}{d^2} - \alpha^2}\left(e^{-\alpha x} - \frac{1 + l_d^2\alpha^2}{\alpha d\left(1 + \frac{l_d^2}{d^2}\right)}e^{-\frac{x}{d}}\right). \qquad (8)$$

Taking into account the deformation parameter $\varepsilon(x)$, the spatial redistribution of defects caused by the self-consistent interaction between the point defects and the deformation field is described by the expression

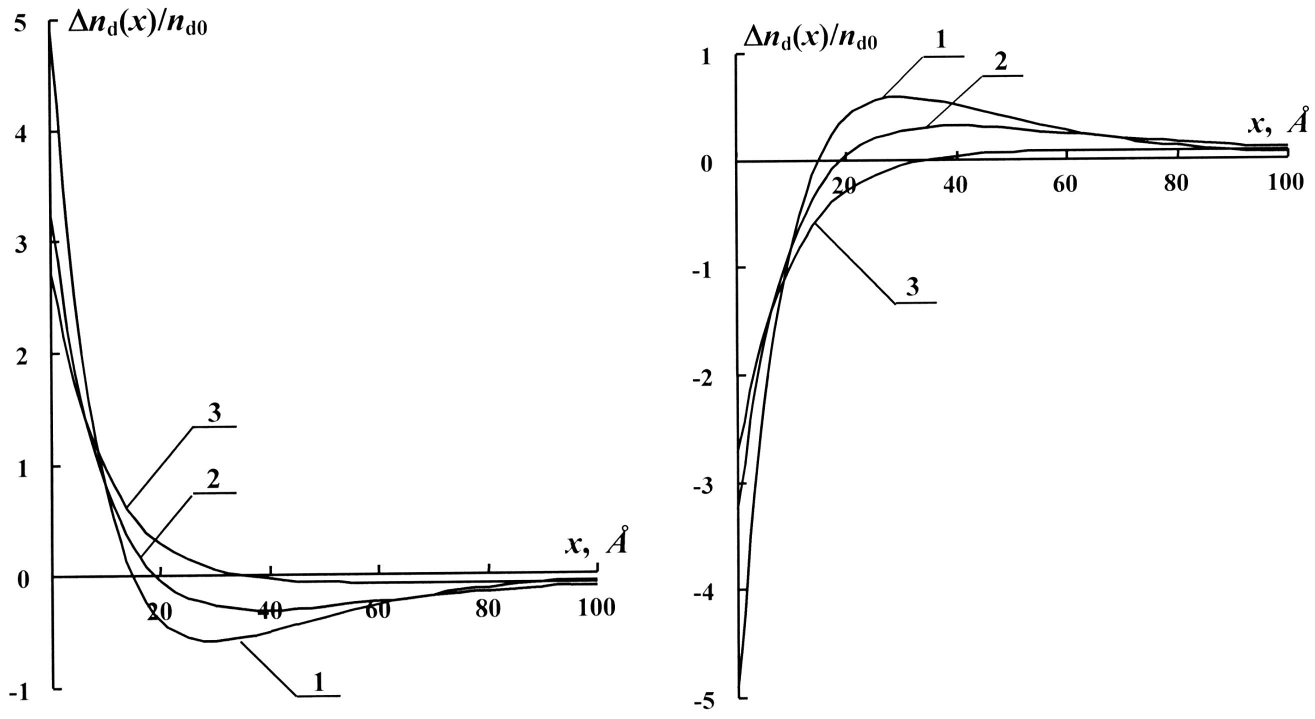
$$n_d(x) = n_{d_0}\left(1 + \frac{\theta_d}{kT}\left(\frac{n_{dc}}{n_{d0}}\frac{\xi_0}{l_d^2}\frac{1}{\frac{1}{d^2} - \alpha^2}\times\right.\right.$$

$$\left.\left.\times\left(\left(1 + l_d^2\alpha^2\right)e^{-\alpha x} - \frac{1 + l_d^2\alpha^2}{\alpha d}e^{-x/d}\right)\right)\right). \qquad (9)$$

In the limit case $x \to \infty$, the deformation $\varepsilon(x) \to 0$ [see Eq. (8)], and the defect concentration approaches the spatially uniform distribution [$n_d(x) \to n_{d0}$, see Eq. (9)]. In the absence of defects ($n_{d0} = 0$), the crystal undergoes a deformation only due to a mismatch of the crystal lattice parameters between the substrate and the epitaxial layer ($\varepsilon(x) = \xi_0 e^{-\alpha x}$).

3. Numerical Calculations and Discussion of Results

The numerical calculations of the deformation parameter and the spatial distribution of defects were carried out for the system InAs/GaAs ($a_s = 5.65$ Å; $a_0 = 6.08$ Å; $C_{11} = 0.833$ Mbar; $C_{12} = 0.453$ Mbar; $\alpha = 0.1$ Å^{-1}; $l_d = 29$ Å; $T = 300$ K; and $\theta_d = 1$ eV).



a

b

Fig. 2. Spatial redistributions of point defects of the tension-center type ($\theta_d > 0$) (*a*) and the compression-center type ($\theta_d < 0$)(*b*) for various average values of the defect concentration $n_{d0} = 0.4n_{dc}$ (*1*), $0.7n_{dc}$ (*2*), and $0.99n_{dc}$ (*3*)

The coordinate, x, dependences of the deformation parameter ε and the relative variation of the defect concentration $\frac{\Delta n_d}{n_{d0}}$ are presented in Figs. 1, 2 for various average concentrations n_{d0} within the interval $0 \le n_{d0} \le n_{dc}$. The dependences $\varepsilon(x)$ and $\frac{\Delta n_d(x)}{n_{d0}}$ are nonmonotonous and possess minima, the positions of which are governed by the average concentration of point defects n_{d0}. As n_{d0} grows, the minima move away from the heterointerface. Such a behavior of those dependences can be understood from the following reasons. Both the deformation parameter ε and the spatial redistribution of point defects $\frac{\Delta n_d}{n_{d0}}$ are determined by two self-consistent competing factors: the component of a deformation that arises due to the mismatch of lattice parameters in the substrate and the epitaxial layer, and the component of deformation induced owing to the spatial redistribution of defects.

There exists such a limit concentration of defects, at which the deformation of the epitaxial layer lattice in the vicinity of the heterointerface changes its sign. Such a phenomenon is observed if the average concentration of defects is in the range $\frac{\alpha^2 l_d^2}{1+\alpha^2 l_d^2} n_{dc} < n_{d0} < n_{dc}$. It can be explained by the fact that the grown layer near the heterointerface becomes either enriched with interstitial atoms at $\theta_d > 0$ (Fig. 2) or depleted of vacancies at $\theta_d < 0$ (Fig. 3). This results in the volume increase of the crystal lattice in comparison with the structure without point defects (Fig. 1, curve *1*). In compressed layers ($a_s^{\mathrm{GaAs}} < a_0^{\mathrm{InAs}}$), impurities ($\theta_d > 0$) are concentrated near the interface (Fig. 2). On the contrary, while moving away from the latter, their concentration decreases. Such an effect was observed in experimental works [4, 5], where the stressed GaAs/InGaAs heterointerfaces were shown to hamper the diffusion of hydrogen and defects into the bulk of the crystal. The opposite scenario is observed for vacancies ($\theta_d < 0$) which are concentrated at a distance of 20—50Å from the heterointerface, while a reduction of the vacancy concentration is observed in the interface vicinity in comparison with the spatially homogeneous distribution.

If the limit concentration is exceeded ($n_{d0} > n_{dc}$), there emerge periodic DD nanostructures in the medium

[2]. It has been shown that their formation is described by the Ginzburg—Landau equation.

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ДЕФОРМАЦІЯ ҐРАТКИ ТА ПРОСТОРОВИЙ ПЕРЕРОЗПОДІЛ ТОЧКОВИХ ДЕФЕКТІВ У НАПРУЖЕНОМУ ЕПІТАКСІЙНОМУ ШАРІ

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Резюме

Побудовано модель деформаційно-дифузійних явищ у напружених епітаксійних шарах на основі самоузгодженої системи рівнянь для концентрації дефектів та параметра деформації. Зроблено розрахунок стаціонарного профілю точкових дефектів (міжвузловинних атомів і вакансій) та параметра деформації ґратки в епітаксійних шарах InAs, вирощених на підкладці GaAs. Показано, що за наявності точкових дефектів у епітаксійному шарі, координатна залежність параметра деформації з віддаленням від гетеромежі носить немонотонний характер.