SURFACES OF ELECTRON DENSITY REDISTRIBUTION IN A ZnSe/GaAs HETEROSTRUCTURE WITH A MISFIT DISLOCATION WALL

R.M. PELESHCHAK, M.M. BARAN[1]

Ivan Franko Drohobych State Pedagogical University
(34, Ivan Franko Str., Drohobych 82100, Ukraine),

[1]**Institute of Business and Innovative Technologies at the Lviv Polytechnic National University**
(18, Horbachevs'kyi Str., Lviv 79044, Ukraine)

UDC 537.226+537.311/0.1

In the framework of the self-consistent electron-deformation model, the surface of the electron concentration distribution near a dislocation wall in a strained ZnSe/GaAs heterosystem has been calculated, and the change of its shape as a function of the average value of the conduction electron concentration and the distance between misfit dislocations has been studied. The profiles of the electron concentration surface have been demonstrated to be sinusoidal-like in the direction parallel to the misfit dislocation line and Gaussian-like in the direction perpendicular to it.

The heterosystem is formed during the epitaxial growth of a layer on a single-crystalline substrate. If the epitaxial layer and the substrate have a mismatch between their lattice parameters a's (for example, in the case ZnSe/GaAs(001)), there emerge elastic deformations and stresses in both contacting media. The structure of the first monoatomic layer of the film accommodates to the substrate lattice in such a manner that the crystalline lattice of the layer duplicates the lattice pattern on the substrate's surface. Several next layers of the film accomodate to the previous ones in precisely the same way. The magnitudes of epitaxial deformations and stresses can be estimated as $\varepsilon \sim (a_{\mathrm{ZnSe}} - a_{\mathrm{GaAs}})/a_{\mathrm{ZnSe}} \approx 4\%$ and $\sigma_i = \mu_i \varepsilon$, respectively, where μ is the modulus of elasticity. As the epitaxial layer grows, the elastic deformation energy increases. Since the elastic energy grows proportionally to the film volume, the further growth of a perfect epitaxial film becomes energetically unfavorable starting from a certain film's thickness. In this case, there appear dislocations in the epitaxial layer near the film–substrate interface [1, 2]. They are aligned in parallel to one another and at approximately identical distances, so that a dislocation wall is formed (Fig. 1). The number of emerged dislocations and their Burgers vectors are sufficient in order that the dislocation deformations compensate the epitaxial ones at large distances from the heterointerface. The distance between neighbor dislocations d is equal to $|\vec{b}|/\varepsilon$, where $|\vec{b}|$ is the corresponding component of the Burgers vector. Owing to the compensation of deformations, the elastic energy becomes localized in a near-surface epitaxial layer of thickness d, and the further growth of the film proceeds without the appearance of structural inhomogeneities. The rate of deformation decay away from the heterojunction is governed by chemical bonds and mismatches between lattice parameters and thermal expansion factors.

The availability of the dislocation wall gives rise to the emergence of mechanical deformation [1, 3]

$$U_{\mathrm{mech}}(|x|, y) = \frac{U_0 \sin(\tilde{\theta}\, y)}{(\mathrm{ch}(\tilde{\theta}\,|\mathrm{x}|) - \cos(\tilde{\theta}\,\mathrm{y}))d}, \qquad (1)$$

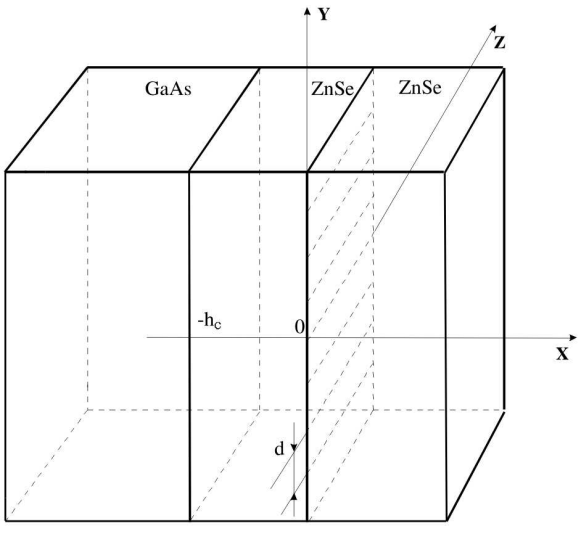

Fig. 1. Schematic presentation of a ZnSe heteroepitaxial layer with an edge dislocation wall grown on the GaAs(001) substrate. Dashed lines designate an edge dislocation wall. Dislocations in the wall are located at a distance d from one another

where $U_0 = \frac{b(1-2\nu)}{2(1-\nu)}$, $\tilde{\theta} = 2\pi/d$, $\vec{b}$ is the Burgers vector directed along the OX axis, ν is Poisson's ratio, and d is the interdislocation distance. As is seen from Eq. (1), such a mechanical deformation is an alternating quantity along the OY axis.

The calculations of the electron concentration redistribution $\Delta n\left(|x|, y\right)$ along the dislocation wall were carried out on the basis of the relation [?]

$$\Delta n\left(|x|, y\right) = R_S\left(e\varphi - SU_{\rm mech}\right), \tag{2}$$

where the potential φ was found from the Poisson equation

$$\varepsilon\nabla^2_{\vec{r}}\varphi\left(\vec{r}\right) - g^2\varphi\left(\vec{r}\right) = aU_{\rm mech}\left(\vec{r}\right), \tag{3}$$

$a = -eR_SS/\varepsilon_0$, and $g^2 = e^2R_S/\varepsilon_0$. The profile $U_{\rm mech}\left(\vec{r}\right)$ was determined by formula (1). Expanding the functions $\varphi\left(\vec{r}\right)$ and $U_{\rm mech}\left(\vec{r}\right)$ into the relevant Fourier integrals

$$\varphi\left(\vec{r}\right) = \frac{\Omega}{\left(2\pi\right)^3}\int\Phi\left(\vec{k}\right)e^{i\vec{k}\vec{r}}d\vec{k},$$

$$U_{\rm mech}\left(\vec{r}\right) = \frac{\Omega}{\left(2\pi\right)^3}\int U_{\rm mech}\left(\vec{k}\right)e^{i\vec{k}\vec{r}}d\vec{k}. \tag{4}$$

and substituting relations (4) into Eq. (3), we obtained the following expression for the potential $\Phi(\vec{k})$ in the $\vec{k}$-space:

$$\Phi(\vec{k}) = -\frac{a}{\varepsilon\,k^2 + g^2}U_{\rm mech}(\vec{k}), \tag{5}$$

where

$$U_{\rm mech}(\vec{k}) = -i\frac{8\pi\tilde{\theta}U_0}{\Omega d}\delta(k_z)\frac{\delta(k_y - \tilde{\theta}) - \delta(k_y + \tilde{\theta})}{\tilde{\theta}^2 + k_x^2} \tag{6}$$

is the Fourier transform of the mechanical part of the deformation parameter $U_{\rm mech}\left(|x|, y\right)$ (see Eq. (1)) at

$$\left|\frac{2\pi}{d}x\right| \gg 1. \tag{7}$$

Carrying out the inverse Fourier transformation, we obtained an analytical expression for the potential $\varphi\left(|x|, y\right)$ in the $\vec{r}$-space:

$$\varphi\left(|x|, y\right) = -\frac{ba\sin\left(\frac{2\pi}{d}y\right)}{dg^2}\frac{1-2\nu}{1-\nu}\times$$

$$\times\left[e^{-2\pi|x|/d} - \frac{2\pi}{d\sqrt{4\pi^2/d^2 + g^2/\varepsilon}}\times\right.$$

$$\left.\times\exp\left(-|x|\sqrt{4\pi^2/d^2 + g^2/\varepsilon}\right)\right]. \tag{8}$$

Substituting expression (8) into Eq. (2) and taking Eqs. (1) and (7) into account, we obtained the formula for the redistribution of electrons $\Delta n\left(|x|, y\right)$ in the vicinity of the wall plane:

$$\Delta n\left(|x|, y\right) = n\left(|x|\right)\sin\left(\frac{2\pi}{d}y\right). \tag{9}$$

It is evident from formula (9) that the electron concentration distribution along the dislocation wall demonstrates the harmonic behavior with the period d along the OY axis and the amplitude

$$n\left(|x|\right) = -\frac{b}{d}\frac{1-2\nu}{1-\nu}SR_S\frac{2\pi}{d\sqrt{4\pi^2/d^2 + g^2/\varepsilon}}\times$$

$$\times\exp\left(-|x|\sqrt{4\pi^2/d^2 + g^2/\varepsilon}\right). \tag{10}$$

In Figs. 2 and 3, the surfaces of the electron concentration distribution in a ZnSe/GaAs(001) heterosystem with a misfit dislocation wall are shown for the average values of the conduction electron concentration $n_0 = 10^{18}$ and 10^{19} cm^{-3}, respectively. The calculations were carried out for the following values of the parameters which correspond to the ZnSe/GaAs(001) heterosystem: $m^* = 0.17m_0$, $S = 3.65$ eV, $a = 5.65$ Å, and $K = 0.379$ eV/Å^3. Panels a correspond to the interdislocation distance $d = 1000$ Å, and panels b to $d = 500$ Å.

From those figures, it is evident that the profile of the electron density surface is sinusoidal-like in the direction parallel to the line, where the misfit dislocations are located (axis OY) and Gaussian-like in the direction perpendicular to the plane that contains the dislocation wall. There is an excess of the electron concentration with respect to its average value in those regions of the crystal lattice which contain dislocation planes. As the degree of the conduction band occupation (within the range of electron concentrations $n_0 = 10^{18} \div 10^{19}$ cm^{-3}) and the interdislocation distance d grow, the redistribution of the electron concentration in the vicinity of dislocations with respect to its average value becomes lower. In particular, if the concentration of conduction electrons becomes an order of magnitude higher (from 10^{18} to 10^{19} cm^{-3}), its maximal relative variation decreases by a factor of about 7 at $d = 1000$ Å and by an order of magnitude at $d = 500$ Å. This is caused by the fact that the crystal lattice becomes less sensitive to deformations if the degree of the conduction band occupation increases [7]. The maxima and minima of the relative variation of the electron

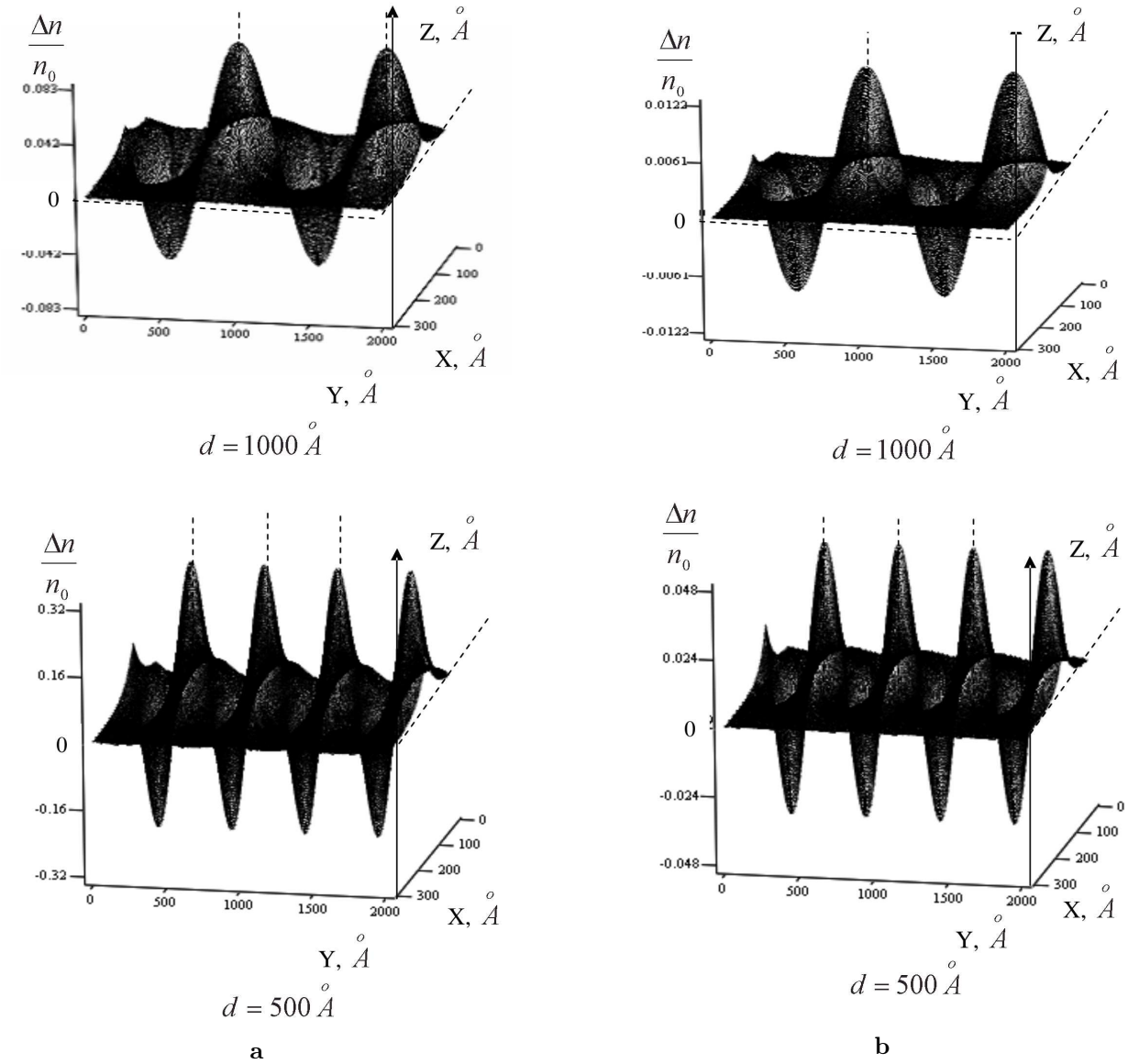

Fig. 2. Surfaces of the electron concentration distribution in the ZnSe/GaAs(001) heterosystem with a misfit dislocation wall for the average concentration of conduction electrons $n_0 = 10^{18}$ (a), 10^{19} cm^{-3} (b) and various interdislocation distances d. Vertical dashed lines correspond to dislocation lines

concentration along the misfit dislocation wall have the ordinates $y_k^{\max} = (4k+1)\,d/4$ and $y_k^{\min} = (4k-1)\,d/4$, respectively. Figures 2 and 3 testify that the width of the region of the conduction-electron spatial localization in a vicinity of the misfit dislocation wall is more sensitive to a variation of the period d than to the degree of conduction band occupation n_0.

To summarize, the results of our researches made it possible to draw the following conclusions:

– the profile of the electron concentration surface is sinusoidal-like in the direction parallel to the misfit dislocation line and Gaussian-like in the direction perpendicular to it;

– if the degree of conduction band occupation n_0 and the interdislocation distance d grow (the former in the interval (10^{18} cm$^{-3} \le n_0 \le 10^{19}$ cm^{-3}), the spatial redistribution of the electron concentration in a vicinity of misfit dislocations with respect to its average value n_0 becomes lower;

– local electron-deformation drains for point defects are formed on dislocations along the dislocation wall, which ultimately leads to a more uniform distribution of point defects in the crystal and to the weakening of degradation effects.

1. Yu.A. Tkhorik and L.S. Khazan, *Plastic Deformation and Misfit Dislocations in Heteroepitaxial Systems* (Naukova Dumka, Kyiv, 1983) (in Russian).
2. L.A. Pastur and E.P. Feldman, Fiz. Tverd. Tela **14**, 2689 (1972).
3. L.D. Landau and E.M. Lifshitz, *Quantum Mechanics. Non-Relativistic Theory* (Pergamon, New York, 1965).
4. R.M. Peleshchak, Preprint ITP AS UkrSSR No. 89-53, Kyiv, 1989 (in Russian).
5. R.M. Peleshchak and M.M. Baran, Funct. Mater. **9**, 474 (2002).
6. L.D. Landau and E.M. Lifshitz, *Theory of Elasticity* (Pergamon, New York, 1959).
7. I.V. Stasyuk and R.A. Grigorchuk, Phys. Status Solidi B **112**, 327 (1982).

Received 11.12.06.
Translated from Ukrainian by O.I. Voitenko

ПОВЕРХНІ ПЕРЕРОЗПОДІЛУ ЕЛЕКТРОННОЇ ГУСТИНИ В ГЕТЕРОСТРУКТУРІ ZnSe/GaAs ЗІ СТІНКОЮ ДИСЛОКАЦІЙ НЕВІДПОВІДНОСТІ

Р.М. Пелещак, М.М. Баран

Р е з ю м е

У рамках самоузгодженої електрон-деформаційної моделі розраховано поверхню електронної густини в околі дислокаційної стінки в напруженій гетеросистемі ZnSe/GaAs та досліджено зміну її форми в залежності від середнього значення концентрації електронів провідності та відстані між дислокаціями невідповідності. Показано, що в напрямку, паралельному лінії розміщення дислокацій невідповідності, форма поверхні електронної густини є синусоподібною, а в напрямку, перпендикулярному до неї, – гаусоподібною.