ROLE OF THE ELECTRON-DEFORMATION INTERACTION IN THE FORMATION OF THE $n - n^+$ JUNCTION IN A DOPED CRYSTAL MATRIX

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In the framework of the electron-deformation model, the criterion of the appearance and the absence of an $n - n^+$ junction in the elastic region of the doped crystal matrix GaAs(100)+Ar(Si) has been established. It has been shown that the more the population of the conduction band ($0 \leq \bar{n} \leq 0.5$), the sharper the $n - n^+$ junction. In this case, the plane corresponding to the junction edge shifts towards the edge of the elastic region.

Introduction

In [1], the experimental research of the influence of the mechanical stresses induced by ionic implantation and grinding of one of the surfaces of gallium arsenide crystals on the redistribution of point defects in a near-surface layer was carried out. The relative change of the lattice parameter, when going towards the depth of the doped crystal matrix, was also calculated in the framework of a mechanical-deformation model. However, the non-uniform deformation, induced by implanted impurities, results in a local change of the electron spectrum, which leads to the spatial redistribution of electrons and the emergence of the electrostatic potential [2, 3].

The purpose of the present work is to study, in the framework of the method of self-consistent electron-deformation relation, the conditions for the $n - n^+$ junction in the doped crystal matrix GaAs(100)+Ar(Si) to appear.

Model

The implantation of impurities into the crystal matrix induces there a non-uniform deformation $U(\mathbf{r}) = \mathrm{Sp}\,\hat{U}(\mathbf{r})$ which results in a local change of the band spectrum. As a consequence, the spatial redistribution of electrons $\Delta n(\mathbf{r})$ takes place, which gives birth to the electrostatic potential $\phi(\mathbf{r})$. To find the electron density $\Delta n(\mathbf{r})$ and the electrostatic potential $\phi(\mathbf{r})$ in the direction of implantation (along the x-axis), it is necessary to solve self-consistently the following system of equations [3]:

1) the stationary Schrödinger equation

$$\left[\nabla^2_{\mathbf{r}} - \frac{S}{\alpha}U(\mathbf{r}) + \frac{e}{\alpha}\phi(\mathbf{r})\right]\Psi_n(\mathbf{r}) =$$

$$= -\frac{1}{\alpha}(\lambda_n - \lambda_0)\,\Psi_n(\mathbf{r}), \qquad (1)$$

where $\alpha = \hbar^2/(2m^*)$, λ_0 is the bottom energy of the conduction band in an undistorted crystal matrix, and S is a constant of the deformation potential of the conduction band;

2) the equation of mechanical equilibrium

$$\left\langle \partial\hat{H}/\partial U(\mathbf{r}_i)\right\rangle = \sigma_{\mathrm{mech}}V, \qquad (2)$$

where

$$\hat{H} = \sum_{i\sigma}[W + SU(\mathbf{r}_i)]c^+_{i\sigma}c_{i\sigma} + \sum_{ij}{}^{/}\sum_{\sigma}\lambda^0_{ij}c^+_{i\sigma}c_{j\sigma} +$$

$$+\frac{1}{2}\sum_i K_A\Omega_0U^2(\mathbf{r}_i) + \hat{H}_{\mathrm{C}},$$

$c^+_{i\sigma}(c_{i\sigma})$ is the Fermi operator of creation (annihilation) of the electron with a spin σ in the localized Wannier state at the i-th lattice point, W is the energy that defines the middle position of the electron energy band; λ^0_{ij} are the transfer integrals in the conduction band of the undistorted lattice, K_A is an elastic constant, Ω_0 is the volume of the unit cell, $\hat{H}_{\mathrm{C}}$ is the energy of the Coulomb interaction between electrons, σ_{mech} is the mechanical strain created by the implanted impurities, and V is the volume of the doped crystal matrix;

3) the equation which determines the concentration of electrons

$$n(\mathbf{r}) = \sum_n \frac{\Psi_n^*(\mathbf{r})\,\Psi_n(\mathbf{r})}{\exp\left(\beta\left(\tilde{\lambda}_n - \mu\right)\right) + 1}, \tag{3}$$

where $\tilde{\lambda}_n = \lambda_n - \lambda_0$;

4) the Poisson equation used to determine the electrostatic potential $\phi(\mathbf{r})$:

$$\nabla^2\phi(\mathbf{r}) = -e\Delta n(\mathbf{r})/(\varepsilon\varepsilon_0), \tag{4}$$

5) the equation for the determination of the chemical potential in the doped crystal:

$$\Omega_0/V \int_V n(r)dr = \bar{n}, \quad 0 \le \bar{n} \le 2, \tag{5}$$

where $\bar{n} = n_0\Omega_0$ is the given average number of electrons at a lattice point.

We consider the doped crystal matrix with a significant average concentration of electrons $n_0 \sim 10^{18} \div 10^{19}$ cm^{-3}. This case can be realized by doping the crystal matrix of GaAs by Si or Ar impurities [1]. Then, the redistribution of conduction electrons caused by the deformation of the doped crystal matrix can lead to the practically full compensation of a deformation shift of the conduction band by the electrostatic interaction energy ($|e\phi| \sim |SU|$) [2]. The wave function in the form of a plane wave is a good solution of the Schrödinger equation (1) in this case.

A change $\Delta n(\mathbf{r}) = n(\mathbf{r}) - n_0$ of the conduction electron concentration in the vicinity of a defect is determined, in the linear approximation, by the relation [3]

$$\Delta n = R_S\left(e\phi - SU_{\text{mech}}\right), \tag{6}$$

where R_S is the function that depends on the electron population in the conduction band, the elastic constants, the effective mass of current carriers, and the constant of the deformation potential of the conduction band.

The deformation caused by the presence of an implanted impurity with nonzero volume is defined as [4]

$$U_{\text{mech}}(x) = k_{\nu_i} N(x)/N_0, \tag{7}$$

where $k_{v_i} = V_i/V_0$, V_i and $N(x)$ are the volume and concentration, respectively, of the doping impurity, and V_0 and N_0 are those of the crystal matrix.

The distribution of the doping impurity $N(x)$ created by gradient diffusion,

$$N(x) = N_r \exp\left(-\upsilon(x - x_0)/D\right), \quad x \ge x_0, \tag{8}$$

where N_r is the impurity concentration in the plane $x = x_0$ which corresponds to the edge of the elastic region, and υ is the surface shift rate upon the implantation by impurities, is adopted as the initial one. In view of (6)–(8), the Poisson equation is of the form

$$\nabla^2\phi(x) - g_S^2\phi(x) = -g_S^2 k_{v_i} S\varepsilon_r \exp\left(-\upsilon(x - x_0)/D\right)/e, \tag{9}$$

$$g_S^2 = e^2 R_S/\varepsilon\varepsilon_0$$

with the boundary conditions

$$\phi(x)\,|_{x\to\infty} = 0,$$

$$\phi(x_0) = \phi_0 = k_{v_i} S\varepsilon_r/\left(e\cdot\left(1 + \upsilon/\left(Dg_S\right)\right)\right); \tag{10}$$

where $\varepsilon_r = N_r/N_0$ is the deformation parameter at the edge of the elastic region. The second boundary condition, $\phi(x_0)$, is chosen as that which ensures the condition of electrical neutrality of the crystal matrix with implanted impurities

$$\int_{V_0} \Delta n(x)\,dV = 0. \tag{11}$$

in the region $x \in [x_0, +\infty)$. The corresponding solution of Eq. (9) is

$$\phi(x) = \left(\phi_0 + k_{v_i} S\varepsilon_r/(e((\upsilon/Dg_s)^2 - 1))\right)\times$$

$$\times \exp(-g_s(x - x_0)) - k_{v_i} S\varepsilon_r\times$$

$$\times \exp(-\upsilon(x - x_0)/D)/(e((\upsilon/Dg_s)^2 - 1)). \tag{12}$$

Expression (12) for the potential of the electrostatic field, created by the redistribution of the electron density, contains two summands. The first one corresponds to the component induced by the electron-deformation interaction. The second one describes the component of the electrostatic field potential which is due to a spatial redistribution of electrons resulting from the action of two opposite effects, namely, the conventional gradient diffusion and mechanical-deformation one. The analysis of formula (12) shows that in the region far from the edge of the elastic one ($x \gg x_0$), the potential $\phi(x)$ goes to zero and, in the close proximity to the edge ($x \to x_0$)

$$\phi(x) \to k_{v_i} S\varepsilon_r/(e\,(1 + \upsilon/Dg_s)). \tag{13}$$

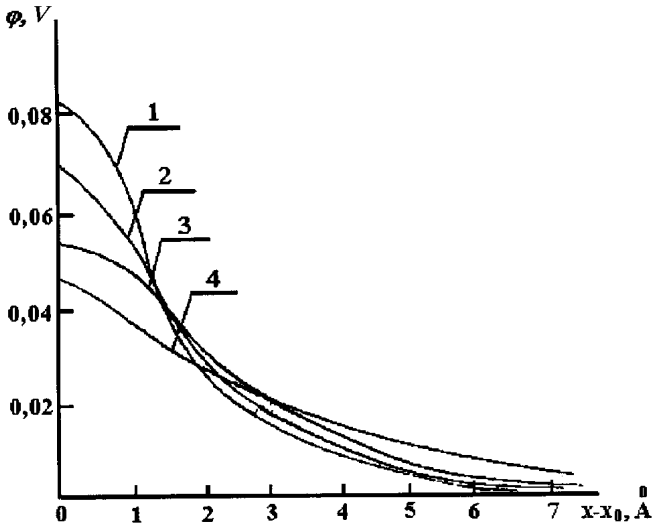

Fig. 1. Coordinate dependences of the electrostatic potential $\phi(x)$ for various populations of the conduction band $\bar{n}$: (*1*) 0.5, (*2*) 0.1, (*3*) 0.01, (*4*) 0.001

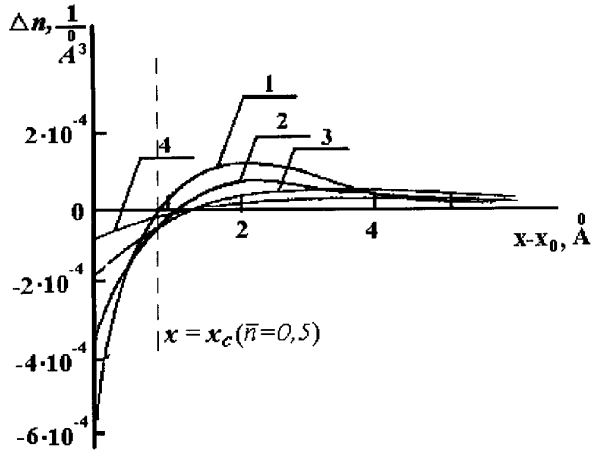

Fig. 2. Coordinate dependences of the electron concentration variation $\Delta n(x)$ for various $\bar{n}$. The notations are the same as in Fig. 1. The dashed line corresponds to the edge of the $n - n^+$ junction

Results of Calculations

The results of numerical calculations of the coordinate dependence of the electrostatic potential $\phi(x - x_0)$ induced by the spatial redistribution of electrons owing to a local change of the conduction band width, which is, in turn, due to the non-uniform deformation of the crystal matrix GaAs(100), doped by Ar(Si) impurity, with the electron-deformation interaction being taken into account, are depicted in Fig. 1. One can see from the figure that, as the population of the conduction band

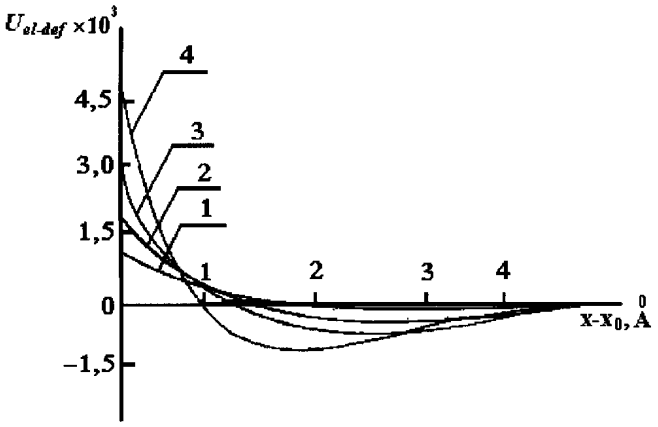

Fig. 3. Coordinate dependences of the electron component of the deformation for various $\bar{n}$. The notations are the same as in Fig. 1

grows within the interval $0 \leq \bar{n} \leq 0.5$, the electrostatic potential in the immediate neighborhood of the edge of the elastic region ($x \geq x_0 + 0$) increases, while the character of this dependence changes to the opposite one at the distances $x \geq x_c(\bar{n})$. Here, $x_c(\bar{n})$ denotes the position of the plane where the concentration change $\Delta n = 0$ (see Fig. 2), i.e. $x_c(\bar{n})$ is the edge of the $n - n^+$ junction.

Such a variation of the potential, as $\bar{n}$ grows within the interval $0 \leq \bar{n} \leq 0.5$, is connected to the fact that the conduction band width in the vicinity of the edge of the elastic region ($x \geq x_0 + 0$) decreases in comparison with that in the region $x \geq x_c(\bar{n})$ due to the opposite character of the electron-deformation component $U_{\mathrm{el-def}} = -S\Delta n\,(x)\,/K_A$ of the deformation in those regions (Fig. 3).

The coordinate dependence of the electrostatic potential $\phi(x)$ for various values of the diffusion coefficient D is shown in Fig. 4. As is seen from the figure, the dependence $\phi(x)$ decreases monotonously as the distance from the edge of the elastic region ($x = x_0$) increases (curves *2* and *3*). The growth of the diffusion coefficient D is accompanied by the increase of the electrostatic potential. In particular, the growth of D by an order of magnitude (curves *3* and *2*) results in the growth of $\phi(x)$ near the edge of the elastic region ($x \geq x_0$) by a factor of two. It is connected to the fact that, as the diffusion coefficient D increases, the distribution of the implanted impurity $N(x)$ in the crystal matrix becomes smoother. At $v/Dg_s \ll 1$, the electrostatic potential of the field (curve *1*) practically does not change along the direction of implantation, because the deformation of the crystal lattice with implanted impurities becomes homogeneous, which results in the

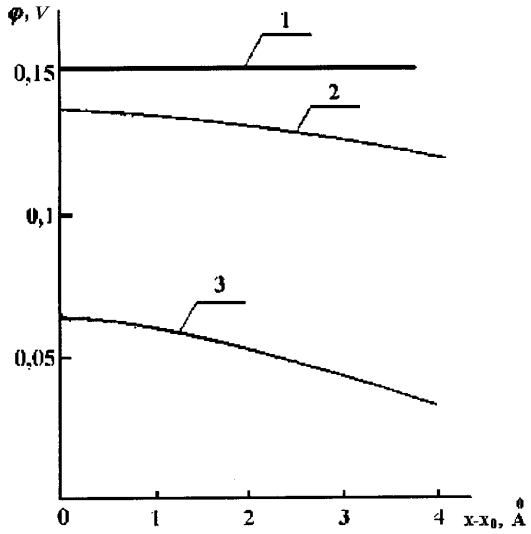

Fig. 4. Dependences $\phi(x)$ for various values of the diffusion coefficient D: (*1*) 10^{-12}, (*2*) 10^{-15}, (*3*) 10^{-16} cm^{-2}/s

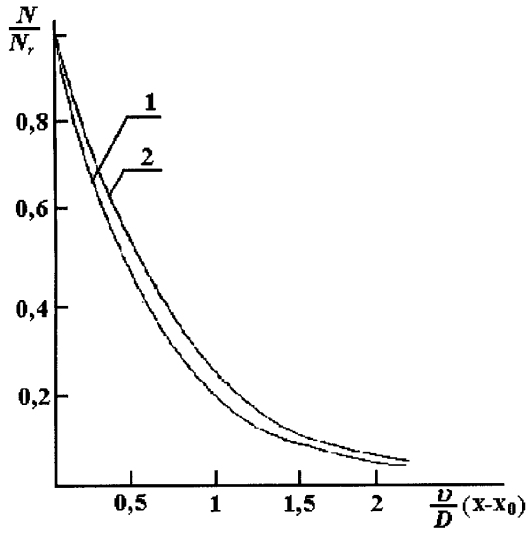

Fig. 5. Coordinate dependences of the doping impurity concentration for $\bar{n} = 0.5$ (*1*) and 0.001 (*2*)

identical energy shift of the bottom of the conduction band in the region $x \geq x_0$. In this case, the appearance of the barrier structure, while doping the crystal matrix by an impurity, becomes impossible.

The analysis of the coordinate dependence of the electron concentration variation $\Delta n(x)$ shows (Fig. 2) that there is a deficiency of electrons in the interval $x_0 < x \leq x_c$ and an excess of them in the region $x > x_c$. Thus, the doping of the crystal matrix of GaAs by Si or Ar impurities results in the formation of a double electrical layer in the elastically deformed region $x_c - d^-(\bar{n}) < x < x_c - d^+(\bar{n})$, where $d^-(\bar{n})$ and $d^+(\bar{n})$ are the effective widths of regions with the electron deficiency and excess, respectively. As the population of the conduction band increases within the interval $0 \leq \bar{n} \leq 0.5$, the profile of the barrier structure $(n - n^+)$ becomes sharper.

As is seen from Fig. 3, the electron component of the deformation $U_{\text{el-def}} = -S\Delta n\,(x)\,/K_A$ additionally stretches the crystal matrix in the elastically deformed region $(x_0 < x \leq x_c)$, and compresses it in the region $x > x_c$, counteracting the mechanical stretching deformation caused by the implanted impurities.

Thus, the total non-uniform deformation $U_{\text{mech}} + U_{\text{el-def}}$, driven by both the purely mechanical and electron-deformation stresses, will affect the diffusion of the impurity. Taking those effects into account, the stationary equation of diffusion will be written down as

$$D\frac{\partial^2 N}{\partial x^2} - \frac{\partial}{\partial x}\left[D\frac{N_0}{N_b}N\frac{\partial}{\partial x}\left(U_{\text{mech}} + U_{\text{el-def}}\right)\right] \times$$

$$\times\Theta\left(N_r - N\right) + \upsilon\frac{\partial N}{\partial x} = 0. \tag{14}$$

The second summand corresponds to a qualitatively new phenomenon, the "flow of the deformation retraction", resulted, in our case, not only from the mechanical component [5], but also the electron component of the deformation. The Heaviside function $\Theta(N_r - N)$ indicates the non-zero value of the latter component in the region of elastic deformations $(N < N_r)$.

Taking into account the boundary conditions $\partial N/\partial x|_{x\to\infty} = N(\infty) = 0$ and $N(x_0) = N_r$, the solution of Eq. (14) is

$$\frac{N}{N_r}\exp\left[K_v a\left(1 + \frac{S^2 R_s}{K_a}\right)\left(1 - \frac{N}{N_r}\right)\right] =$$

$$= \exp\left(-\frac{\upsilon}{D}\left(x - x_0\right)\right)\exp\left[-k_{v_i}a\frac{S^2 R_s}{K_a}\times\right.$$

$$\times\left(\frac{\upsilon/(Dg_s)}{\upsilon^2/(D^2 g_s^2) - 1}e^{-g_s(x-x_0)} -\right.$$

$$\left.\left. - \frac{1}{\upsilon^2/(D^2 g_s^2) - 1}e^{-\frac{\upsilon}{D}(x-x_0)} - \frac{1}{1 + \upsilon/(Dg_s)}\right)\right], \tag{15}$$

where $a = \frac{N_0}{N_b}\varepsilon_r$, $N_b = N_0\frac{kT(1-2\nu_1)\rho}{W_0(1-\nu_1)r_1}$, W_0 is the height of the diffusion barrier, r_1 is the characteristic radius of the diffusion channel, ρ is the constant entering the expression for the model potential $V(r) \sim \exp(-r/\rho)$ [5].

The coordinate distributions of the impurities for two values of the population of the electron energy band are shown in Fig. 5. It is noticeable that the larger the electron population of the conduction band, the more localized the profile of the impurity distribution in the vicinity of the edge of the elastic region. It is connected to the fact that, as the population $\bar{n}$ in the conduction band grows, the contribution of the electron-deformation flow, which is opposite to the gradient one, to the diffusion process increases [3].

Thus, on the basis of the obtained results, it is possible to make the following conclusions:

i) Provided that $v/(Dg_s) \geq 1$, where v is the shift rate of the crystal surface, when the crystal is being doped with impurities, D is the diffusion coefficient, and $g_s^2 = e^2 R_s/(\varepsilon\varepsilon_0)$, an $n - n^+$ junction appears in the elastic region of the doped crystal matrix GaAs+Ar(Si). In the case $v/(Dg_s) \geq 1$, such a junction is absent.

ii) As the population of the conduction band grows within the interval $0 \leq \bar{n} \leq 0.5$, the electrostatic potential increases in the region from the edge $x = x_c(\bar{n})$ of the $n - n^+$ junction to the edge of the elastic region $x = x_0$, and falls down beyond it.

iii) The electron-deformation interaction additionally stretches the crystal matrix near the edge of the elastic region and compresses it beyond the plane $x = x_c$ which corresponds to the edge of the $n - n^+$ junction.

The availability of the $n - n^+$ junction in the doped crystal matrix GaAs+Ar(Si) should reveal itself upon the measurements of current-voltage characteristics.

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РОЛЬ ЕЛЕКТРОН-ДЕФОРМАЦІЙНОЇ ВЗАЄМОДІЇ В УТВОРЕННІ $n - n^+$-ПЕРЕХОДУ В ІМПЛАНТОВАНІЙ КРИСТАЛІЧНІЙ МАТРИЦІ

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Р е з ю м е

В рамках електрон-деформаційної моделі встановлений критерій виникнення $n - n^+$-переходу та його відсутності в пружній області імплантованої кристалічної матриці GaAs(100)+Ar(Si). Показано, що з ростом ступеня заповнення зони провідності ($0 \leq \bar{n} \leq 0,5$) $n - n^+$-перехід стає більш різким. При цьому площина, що відповідає межі переходу, з ростом $\bar{n}$ зміщується до межі пружності.