Functional Materials 12, No.2 (2005) © 2005 — Institute for Single Crystals

The formation of n–n^+ transition in the implanted crystal matrix

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Received February 8, 2004

The existence of n–n^+ transition in the elastic area of the implanted crystal matrix GaAs(100) + Ar(Si) is discussed within the framework of the electron-deformation model. It is shown that n–n^+ transition becomes sharper with the increase of conductivity zone population ($0 \le \bar{n} \le 0.5$). Thus the plane, which corresponds to the border of transition, is shifted to the border of elasticity with the increase of $\bar{n}$.

В рамках электрон-деформационной модели раскрыто существование n–n^+ перехода в упругой области имплантированной кристаллической матрицы GaAs(100) + Ar(Si). Показано, что с ростом степени заполнения зоны проводимости ($0 \le \bar{n} \le 0,5$) переход становится более резким. При этом плоскость, соответствующая границе перехода, с ростом $\bar{n}$ сдвигается к границе упругости.

To create materials with given physical properties [1] it is important to predict the implanted admixture distribution profile in the crystal matrix. Along with the information on the admixture distribution, the information on self-consistent electrons and electrostatic potential distribution in the implanted crystal matrix is very important.

The aim of our work is the theoretic study on the nature of electrons redistribution and the change of electrostatic potential in the implanted crystal matrix (GaAs(100) + Ar(Si)). Their nature is caused by diffusionally electron-deformation effects.

Impurities implantation causes the inhomogeneous deformation $U(\mathbf{r}) = Sp\hat{U}(\mathbf{r})$ in the crystal matrix. The deformation, in it turn, leads to the local change of zone spectra. This results in space redistribution of the electrons $\Delta n(\mathbf{r})$, which causes the electrostatic potential $\varphi(\mathbf{r})$ to arise.

To find the electron density $\Delta n(\mathbf{r})$ and electrostatic potential $\varphi(\mathbf{r})$ in the implantation direction (along OX axis) one should solve the following equations set in coordination [2]:

1) Schrodinger stationary equation

$$\left[\nabla_{\mathbf{r}}^2 - \frac{S}{\alpha}U(\mathbf{r}) + \frac{e}{\alpha}\varphi(\mathbf{r})\right]\Psi_n(\mathbf{r}) = -\frac{1}{\alpha}(\lambda_n - \lambda_0)\Psi_n(\mathbf{r}), \quad (1)$$

where $\alpha = \hbar^2/2m^*$, λ_0 is the energy of the conduction band bottom in non-deformed crystal matrix, S is the constant of the conduction band deformation potential;

2) the mechanic equilibrium equation

$$<\frac{\partial \hat{H}}{\partial U(\bar{r}_i)}> = \sigma_{mech}V, \quad (2)$$

where

$$\hat{H} = \sum_{i\sigma}[W + SU(\mathbf{r})]c_{i\sigma}^{+}c_{i\sigma} + \sum_{ij}\sum_{\sigma}\lambda^0{}_{ij}c_{i\sigma}^{+}c_{j\sigma} + \frac{1}{2}\sum_i K_A\Omega_0U^2(\mathbf{r}) + \hat{H}_{coul},$$

$c_{i\sigma}^{+}(c_{i\sigma})$ are the Fermi-operators of birth (destruction) for the electrons with σ spin in

localized Vanier state in junction i; W is the energy which defines the position of electron zone middle; λ_{ij}^0 are the integrals of transition in the conductivity zone of non-deformed lattice, K_A is the elasticity constant, Ω_0 is the volume of an elementary cell; $\hat{H}_{coul}$ is the energy of Coulomb interaction between the electrons, σ_{mech} is the mechanical stress, created by the implanted additives; V is the volume of the implanted crystal matrix;

3) the equation for the electrons concentration $n(\mathbf{r})$

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

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

4) Poisson's equation to determine the electrostatic potential

$$\nabla^2\varphi(\mathbf{r}) = \frac{-e}{\varepsilon\varepsilon_0}\Delta n(\mathbf{r}) \qquad (4)$$

and the equation for finding the chemical potential in the implanted crystal

$$\frac{\Omega_0}{V}\int_V n(\mathbf{r})d\mathbf{r} = \bar{n}, \quad 0 \le \bar{n} \le 2, \qquad (5)$$

where $\bar{n}$ is the given average number of electrons in a junction.

In our problem the case of implanted crystal matrix with a sizable average concentration of conductivity electrons ($n_0 \ge 10^{19}$ cm^{-3}) is considered. This case can be realized if the crystal matrix GaAs is implanted with Ar [1] or Si [2] additives. Then the redistribution of conductivity electrons, resulting from the deformation of the implanted crystal matrix, can lead to virtually full compensation of conductivity zone deformation displacement by electrostatic interaction energy ($|e\varphi| \sim SU$). In this case, a wave function in the form of plane wave is a good approximate solution of the Schrodinger equation (1). This condition can be realized at high initial (in not completely formed state) concentrations of electrons, which is characteristic for semiconductors with high doping level. The redistribution of electrons, due to the displacement and local breadth change of conductivity zone at nonhomogenous deformation, leads to considerable charge accumulation, and the energy of electrostatic interaction becomes of the same order as the deformation energy SU [3].

In the linear approximation, the change of conductivity electrons concentration about the defect $\Delta n(\mathbf{r}) = n(\mathbf{r}) - n_0$ is determined by the following relation [3]

$$\Delta n = R_S(e\varphi - SU_M),$$

$$R_s = \left(\frac{3}{8}\right)^{1/3}\frac{1}{\alpha\pi^{4/3}}\frac{n^{1/3}\left(1 + \frac{S^2n^{1/3}}{(3\pi^2)^{2/3}\alpha K_A}\right)^{1/2}}{1 - \left(\frac{3}{8}\right)^{1/3}\frac{S^2n^{1/3}}{\pi^{4/3}\alpha K_A}\left(1 + \frac{S^2n^{1/3}}{(3\pi^2)^{2/3}\alpha K_A}\right)^{1/2}}. \qquad (6)$$

The deformation that appears due to nonzero volume of the implanted additive is determined as follows [4]:

$$U_M(x) = k_{v_i}\frac{N(x)}{N_0}, \qquad (7)$$

where $k_{v_i} = V_i/V_0$; V_i, $N(x)$, V_0, N_0 are respectively the volume and concentration of the doped additive and crystal matrix atoms.

We recognize the initial distribution of the implanted additives $N(x)$ as the distribution, created by gradient diffusion:

$$N(x) = N_r e^{-\frac{\upsilon}{D}(x - x_0)}, \quad x \ge x_0, \qquad (8)$$

where N_r is the additive concentration in the plane $x = x_0$, which corresponds to the elasticity limit, υ is the rate of crystal surface displacement during the implantation with additives. If we take into account (6), (7), (8) Poisson equation becomes the following:

$$\nabla^2\varphi(x) - g_S^2\varphi(x) = -g_S^2\frac{k_{v_i}S\varepsilon_r}{e}e^{-\frac{\upsilon}{D}(x - x_0)}, \qquad (9)$$

$$g_S^2 = \frac{e^2R_S}{\varepsilon\varepsilon_0}$$

with boundary conditions

$$\begin{cases} \varphi(x)|_{x\to\infty} = 0, \\ \varphi(x_0) = \varphi_0 = \frac{k_{v_i}S\varepsilon_r}{e}\cdot\frac{1}{1 + \frac{\upsilon}{Dg_S}}, \end{cases} \qquad (10)$$

where $\varepsilon_r = N_r/N_0$ is the deformation parameter at the elasticity limit.

The second boundary condition $\varphi(x_0)$ is chosen so that in the region $x \in [x_0;+\infty)$ the condition of crystal matrix electroneutrality with the implanted additives is true:

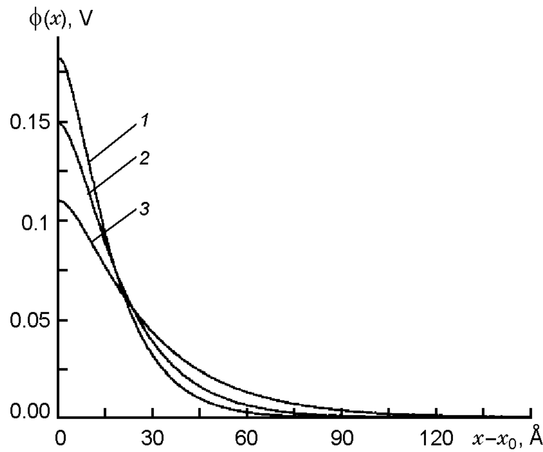

Fig. 1. The coordinate dependence of electrostatic potential $\varphi(x)$ at different values of conductivity zone population $\bar{n}$: *1* — $\bar{n}$ = 0.5; *2* — 0.1; *3* — 0.01.

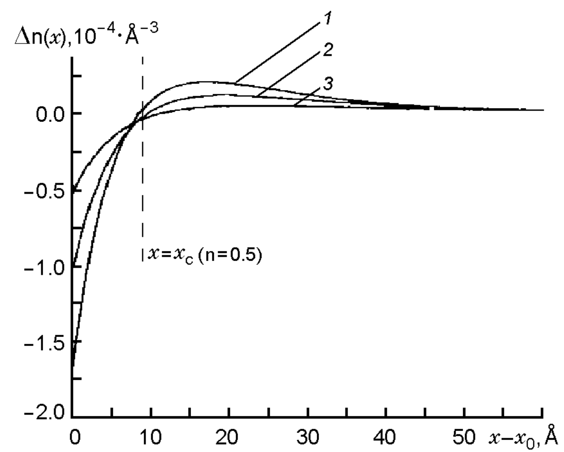

Fig. 2. The coordinate dependence of electrons concentration change $\Delta n(x)$ at different $\bar{n}$: *1* — 0.5; *2* — 0.1; *3* — 0.01; hatch marks the boundary $x = x_c(\bar{n})$ of n–n^+ transition.

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

Having solved the equation (9), we obtain:

$$\varphi(x) = \left(\varphi_0 + \frac{k_{\nu_i} S \varepsilon_r}{e\left(\left(\frac{\upsilon}{Dg_s}\right)^2 - 1\right)}\right)\exp(-g_s(x - x_0)) - \frac{k_{\nu_i} S \varepsilon_r}{e\left(\left(\frac{\upsilon}{Dg_s}\right)^2 - 1\right)}\exp(-\frac{\upsilon}{D}(x - x_0)). \tag{12}$$

The expression (12) for the electrostatic field potential, created by the redistribution of electron density, consists of two items. The first item corresponds to the potential component, determined by electron deformation interaction. The second item describes the component of electrostatic field, created by spatial redistribution of the electrons due to two effects with opposite directions: ordinary gradient diffusion and mechanic-deformation diffusion. The analysis of formula (12) shows that in the region of crystal matrix, distant from the elasticity threshold ($x >> x_0$), $\varphi(x)$ potential tends to zero.

The results coordinate dependency numerical computations for the electrostatic potential $\varphi(x - x_0)$, specified by the spatial redistribution of the electrons due to the local change of conductivity zone breadth at nonhomogenous deformation of the matrix GaAs(100) lattice implanted with the additives Ar(Si), taking into account electron-deformation interaction, are obtained at the following values of the parameters: S = 7.17 eV; ε_r = 0.08; K_A = 0.49 eV/Å^3; ε = 12.8; α = 54.3 eV·Å^2; Ω_0 = 180 Å^3; D = 6 Å^2/c; υ = 1 Å/c [5] and shown in Fig. 1. As one can see, with the increase of conductivity zone population in the interval $0 \le \bar{n} \le 0.5$ the electrostatic potential in immediate proximity to the elasticity boundary ($x \ge x_0 + 0$) increases, and at the distances $x \ge x_c(\bar{n})$ the nature of this dependence changes to the opposite. $x_c(\bar{n})$ is a plane, in which the change of concentration is $\Delta n = 0$ (Fig. 2), that is, it is the boundary of n–n^+ transition.

Such potential change along with the increase of $\bar{n}$ in the interval $0 \le \bar{n} \le 0.5$ is connected with the fact that near the elasticity boundary ($x \ge x_0$) the energetic breadth of conductivity zone becomes narrower compared to the breadth of conductivity zone in the region $x \ge x_c(\bar{n})$ due to the opposite character of electron-deformation component in the deformation ($\Delta U_{el\text{-}def} = -S \cdot \Delta n(x)/K_A$) in these regions (Fig. 3).

The analysis of coordinative dependence of electron concentration change $\Delta n(x)$ shows (Fig. 2) that in the neighborhood $x_0 < x \le x_c$ there is a lack of current carriers, and in the region $x > x_c$ there is surplus of them. So, the implantation of crystal matrix GaAs by the Si or Ar additives causes the formation of double electric layer in elastically deformed region ($x_C - d^-(\bar{n}) < x < x_C + d^+(\bar{n})$), where $d^-(\bar{n})$, $d^+(\bar{n})$ are respectively the effective breadth of the region with the lack

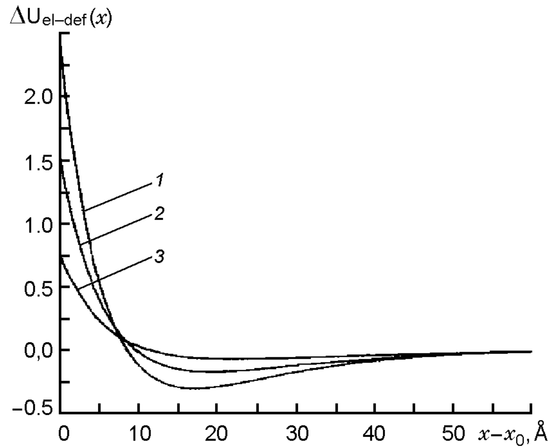

Fig. 3. The coordinate dependence of electron deformation component at different $\bar{n}$: *1* — 0.5; *2* — 0.1; *3* — 0.01.

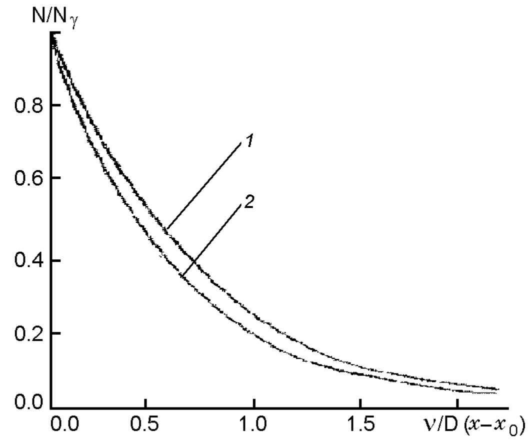

Fig. 4. The coordinate dependence of implanted additive concentration at *1* — $\bar{n}$ = 0.5; *2* — $\bar{n}$ = 0.001.

and surplus of electrons. With the increase of conductivity zone population in the interval $0 < \bar{n} < 0.5$ the region of barrier structure $(n - n^+)$ becomes more abrupt.

Fig. 3 shows that in elastically deformed region $(x_0 < x \le x_c)$ the electron component of deformation $(\Delta U_{el\text{-}def} = -S \cdot \Delta n(x)/K_A)$ restretches the crystal matrix, and in $x > x_c$ region squeezes it, which counteracts the mechanical deformation of stretching, caused by the implanted additives.

So, the summary nonhomogenous deformation $U_{mech} + \Delta U_{el\text{-}def}$, caused by purely mechanical as well as electron-deformation strains, will influence the diffusion of the additive. Taking into account these effects, we can write the stationary diffusion equation in the following form:

$$D\frac{\partial^2 N}{\partial x^2} - \frac{\partial}{\partial x}\left[D\frac{N_0}{N_b}N\frac{\partial}{\partial x}\left(U_{mech} + U_{el-def}\right)\right] \times \theta(N_r - N) + \upsilon\frac{\partial N}{\partial x} = 0. \quad (13)$$

The second item characterizes the qualitatively new phenomenon — "deformation retraction streaming", which is caused, in our case, by not only mechanical [6], but also electron component of the deformation. Heavyside function $(\theta(N_r - N)$ shows that this item is nonzero in the region of elastic deformations $(N < N_r)$.

Taking into account the boundary conditions $\frac{\partial N}{\partial x}|_{x \to \infty} = N(\infty) = 0$ and $N(x_0) = N_r$, we obtain the solution of the equation (13):

$$\frac{N}{N_r}\exp\left[K_v a\left(1 + \frac{S^2 R_s}{K_a}\right)\left(1 - \frac{N}{N_r}\right)\right] = \quad (14)$$

$$= \exp\left(-\frac{\upsilon}{D}(x - x_0)\right)\exp\left[-K_v a\frac{S^2 R_s}{K_a}\left(\frac{\frac{\upsilon}{Dg_s}}{\frac{\upsilon^2}{D^2 g_s^2} - 1}e^{-g_s(x - x_0)} - \frac{1}{\frac{\upsilon^2}{D^2 g_s^2} - 1}e^{-\frac{\upsilon}{D}(x - x_0)} - \frac{1}{1 + \frac{\upsilon}{Dg_s}}\right)\right].$$

In Fig. 4 we can see the additives distribution coordinate dependence on the electron zone population. One can notice that the higher the conductivity zone is populated by electrons, the more the potential profile of additives distribution is localized to the elasticity boundary. This is connected with the fact that the increase of conductivity zone $\bar{n}$ population increases the contribution of electron-deformation streaming, opposite in the direction to the gradient one [3], into the diffusion process.

So, basing on the results obtained, we can make the following conclusions:

1) in the elastic region of the implanted crystal matrix GaAs Ar(Si) transition appears;

2) it is established that while the population of conductivity zone $(0 \le \bar{n} \le 0.5)$ in the region between the boundary $(x = x_c(\bar{n}))$ of n–n^+ transition and the elasticity boundary $(x = x_0)$ increases, the electrostatic potential increases, but beyond this region it decreases;

3) it is shown that in immediate proximity to the $(x \ge x_0)$ boundary the electron-deformation influence restretches the crystal

matrix, but beyond the plane $x = x_c$, which corresponds to boundary of n–n^+ transition it squeezes the matrix.

The presence of n–n^+ transition in the implanted crystal matrix GaAs Ar(Si) should exhibit at the current-voltage characteristics measuring.

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Утворення n–n^+ переходу в імплантованій кристалічній матриці

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У рамках електрон-деформаційної моделі розкрито існування n–n^+ переходу в пружній області імплантованої кристалічної матриці GaAs(100) + Ar(Si). Показано, що із зростанням ступеня заповнення зони провідності ($0 \le \overline{n} \le 0,5$) перехід стає більш різким. При цьому площина, яка відповідає межі переходу, зі зростанням $\overline{n}$ зсувається до межі пружності.