# Decreasing Of Quantity Of Radiation DeFects In Implanted-Junction HeterorecTifiers By Using Overlayers

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**ABSTRACT** 

Recently we introduced an approach to increase sharpness of diffusion-junction and implanted-junction heterorectifiers. The heterorectifiers could by single and as a part of heterobipolar transistors. However manufacturing p-n-junctions by ion implantation leads to generation of radiation defects in materials of heterostructure. In this paper we introduce an approach to use an overlayer and optimization of annealing of radiation defects to decrease quantity of radiation defects.

#### **KEYWORDS**

Implanted-junction heterorectifiers, decreasing of quantity of radiation defects, overlayers

#### **1. INTRODUCTION**

In the present time degree of integration of elements of integrated circuits (such as *p*-*n*-junctions, field-effect and bipolar transistors, thyristors) increases [1-8]. The increasing of degree of integration leads to decreasing of dimensions of elements of integrated circuits. To decrease dimensions of elements of integrated circuits could be used some approaches [9-15]. At the same time with decreasing of dimensions of elements of integrated circuits attracted an interest increasing of quality of solid state electronic materials [16-20].

It has been recently shown (see, for example, [13-15,21]), that manufactured by diffusion or ion implantation *p*-*n*-junctions and bipolar transistors in heterostructures gives us possibility to increase sharpness of the *p*-*n*-junctions. However manufacturing implanted-junction rectifiers leads to generation of radiation defects. In this paper we consider described in the Ref. [21] heterostructure, which consist of a substrate and one or two epitaxial layers (see Figs. 1 and 2).

We assume that type of conductivity of the substrates is known (n or p). We also assume that a dopant is implanted into one of the epitaxial layers for generation into the layer required type of conductivity (p or n). In the first case (see Fig. 1) the dopant is implanted into the single epitaxial layer. In the second case (see Fig. 2) the dopant is implanted into the nearest to the substrate layer of heterostructure. At the same time we assume, that type of conductivity of the external epitaxial layer (see Fig. 2) coincides with type of conductivity of the substrate. Farther we consider annealing of radiation defects. This paper is about analytical modeling redistribution of dopant and radiation defects and analysis the distribution. We solved our aim by analytical calculation distributions of concentrations of dopant and radiation defects. We also consider a modification of recent-

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International Journal on Computational Sciences & Applications (IJCSA) Vol.4, No.2, April 2014 ly introduce analytical approach to solve boundary problems to decrease quantity of iteration steps.

# 2. Method of solution

To model redistribution of dopant let us consider the second Fick's law [1,3-5]

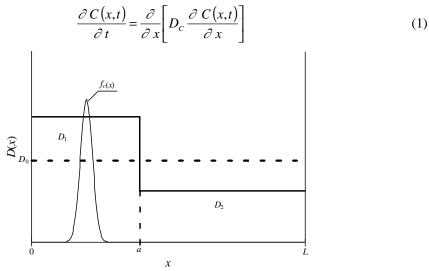


Fig. 1. Heterostructure, which consist of a substrate and an epitaxial layer. The figure also shows initial distribution (before starting of annealing of radiation defects) if implanted dipant

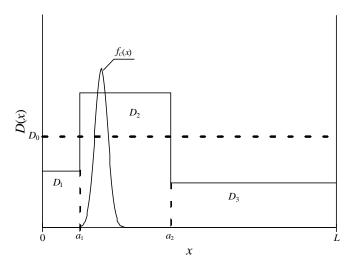


Fig. 2. Heterostructure, which consist of a substrate and two epitaxial layers. The figure also shows initial distribution (before starting of annealing of radiation defects) if implanted dopant with boundary and initial conditions

$$\frac{\partial C(x,t)}{\partial x}\Big|_{x=0} = 0, \ \frac{\partial C(x,t)}{\partial x}\Big|_{x=L} = 0, \ C(x,0) = f(x).$$
(2)

Here C(x,t) is the spatio-temporal distribution of concentration of dopant; *T* is the temperature of annealing; *D* is the dopant diffusion coefficient. Values of dopant diffusion coefficient are differ from each other in different materials of heterostructure. Values of dopant diffusion coefficient

International Journal on Computational Sciences & Applications (IJCSA) Vol.4, No.2, April 2014 also changing with variation of temperature (with account Arrhenius law), after radiation processing and in high-doping case. We approximate dependences of dopant diffusion coefficient on parameters by the following function based on the following references [22-24]

$$D_{c} = D_{L}(x,T) \left[ 1 + \xi \frac{C^{\gamma}(x,t)}{P^{\gamma}(x,T)} \right] \left[ 1 + \zeta_{1} \frac{V(x,t)}{V^{*}} + \zeta_{2} \frac{V^{2}(x,t)}{(V^{*})^{2}} \right],$$
(3)

Here  $D_L(x,T)$  and P(x,T) are the spatial and temperature dependences of dopant diffusion coefficient and limit solubility of dopant. Reason of spatial dependence of the above functions is presents one or more epitaxial layers in the heterostructure. Reason of temperature dependence of the diffusion coefficient and limit of solubility is the Arrhenius law. Values of parameter  $\gamma$  are different in different materials and could be integer in the following interval  $\gamma \in [1,3]$  [22]. V(x,t) is the spatio-temporal distribution of concentration of radiation vacancies;  $V^*$  is the equilibrium distribution of vacancies. Concentrational dependence of dopant diffusion coefficient is described in details in [22]. We determine spatio-temporal distributions of concentrations of point radiation defects by solving the following system of equations [23,24]

$$\begin{cases} \frac{\partial I(x,t)}{\partial t} = \frac{\partial}{\partial x} \left[ D_{I}(x,T) \frac{\partial I(x,t)}{\partial x} \right] - k_{I,I}(x,T) I^{2}(x,t) - k_{I,V}(x,T) I(x,t) V(x,t) \\ \frac{\partial V(x,t)}{\partial t} = \frac{\partial}{\partial x} \left[ D_{V}(x,T) \frac{\partial V(x,t)}{\partial x} \right] - k_{V,V}(x,T) V^{2}(x,t) - k_{I,V}(x,T) I(x,t) V(x,t) \end{cases}$$
(4)

with initial

$$\rho(x,0) = f_{\rho}(x) \tag{5a}$$

and boundary conditions

$$\frac{\partial \rho(x,t)}{\partial x}\Big|_{x=0} = 0, \ \frac{\partial \rho(x,t)}{\partial x}\Big|_{x=L} = 0.$$
(5b)

Here  $\rho=I,V$ . We denote the spatio-temporal distribution of concentration of interstitials as I(x,t). We denote the diffusion coefficients of point radiation defects  $D_{\rho}(x,T)$ . Terms  $V^2(x,t)$  and  $I^2(x,t)$  correspond to generation of divacancies and diinterstitials. We denote the parameters of recombination of point radiation defects and generation of their complexes as  $k_{I,V}(x,T)$ ,  $k_{LI}(x,T)$  and  $k_{V,V}(x,T)$ .

We determine spatio-temporal distributions of concentrations of divacancies  $\Phi_V(x,t)$  and diinterstitials  $\Phi_l(x,t)$  by solution of the following system of equations [23,24]

$$\begin{cases} \frac{\partial \Phi_{I}(x,t)}{\partial t} = \frac{\partial}{\partial x} \left[ D_{\Phi I}(x,T) \frac{\partial \Phi_{I}(x,t)}{\partial x} \right] + k_{I,I}(x,T) I^{2}(x,t) - k_{I}(x,T) I(x,t) \\ \frac{\partial \Phi_{V}(x,t)}{\partial t} = \frac{\partial}{\partial x} \left[ D_{\Phi V}(x,T) \frac{\partial \Phi_{V}(x,t)}{\partial x} \right] + k_{V,V}(x,T) V^{2}(x,t) - k_{V}(x,T) V(x,t) \end{cases}$$
(6)

with boundary and initial conditions

$$\frac{\partial \Phi_{\rho}(x,t)}{\partial x}\Big|_{x=0} = 0, \ \frac{\partial \Phi_{\rho}(x,t)}{\partial x}\Big|_{x=L} = 0, \ \Phi_{I}(x,0) = f_{\Phi I}(x), \ \Phi_{V}(x,0) = f_{\Phi V}(x).$$
(7)

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International Journal on Computational Sciences & Applications (IJCSA) Vol.4, No.2, April 2014 We denote the diffusion coefficients of simplest complexes of point radiation defects  $D_{\phi\rho}(x,T)$ . We denote the parameters of decay of complexes of point defects  $k_{\rho}(x,T)$ .

We calculate spatio-temporal distribution of concentration of dopant by using method of averaging of function corrections [13-15,21,25] with decreased quantity of iteration steps [26]. We used the following functions as initial-order approximations of considered concentrations

Framework the approach we used distributions of concentrations of dopant and radiation defects with averaged values of dopant diffusion coefficient  $D_{0L}$ ,  $D_{0L}$ ,  $D_{0V}$ ,  $D_{0\phi l}$ ,  $D_{0\phi V}$  and zero values of parameters of recombination of defects, generation and decay of their complexes as the initial-order approximations of solutions of Eqs. (1), (4) and (6). The initial-order approximations could be written as

$$C_{1}(x,t) = \frac{1}{L} + \frac{2}{L} \sum_{n=1}^{\infty} F_{nC}c_{n}(x)e_{nC}(t), \quad I_{1}(x,t) = \frac{1}{L} + \frac{2}{L} \sum_{n=1}^{\infty} F_{nI}c_{n}(x)e_{nI}(t), \quad V_{1}(x,t) = \frac{1}{L} + \frac{2}{L} \sum_{n=1}^{\infty} F_{nV}c_{n}(x)e_{nV}(t),$$

$$\Phi_{I1}(x,t) = \frac{1}{L} + \frac{2}{L} \sum_{n=1}^{\infty} F_{n\Phi_{I}}c_{n}(x)e_{n\Phi_{I}}(t), \quad \Phi_{V1}(x,t) = \frac{1}{L} + \frac{2}{L} \sum_{n=1}^{\infty} F_{n\Phi_{V}}c_{n}(x)e_{n\Phi_{V}}(t),$$

where  $F_{n\rho} = \int_{0}^{L} c_n(u) f_{\rho}(u) du$ ;  $e_{n\rho}(t) = \exp(-\pi^2 n^2 D_{0\rho} t/L^2)$ ;  $c_n(\chi) = \cos(\pi n \chi/L)$ ;  $D_{0L}$ ,  $D_{0I}$ ,  $D_{0V}$ ,

 $D_{0, \Phi l}$ ,  $D_{0, \Phi V}$  are the averaged values of diffusion coefficients. Approximations of the second- and higher orders of dopant and defect concentrations we determine framework standard procedure of method of averaging of function corrections [13-15, 21,25,26]. Framework the approach to determine the *n*-th order approximations of the required concentrations we replace the functions C(x,t), I(x,t),  $\Psi_I(x,t)$ ,  $\Phi_I(x,t)$  and  $\Phi_V(x,t)$  on the sum of average value of the *n*-th order approximations and approximations of the *n*-1-th orders, i.e.  $\alpha_{n\rho} + \rho_{n-1}(x,t)$ . In this situation relations of the second-order approximations of the required concentrations could be written as

$$\frac{\partial C_2(x,t)}{\partial t} = \frac{\partial}{\partial x} \left( D_L(x,T) \left[ 1 + \varsigma_1 \frac{V(x,t)}{V^*} + \varsigma_2 \frac{V^2(x,t)}{(V^*)^2} \right] \left\{ 1 + \xi \frac{[\alpha_{2C} + C_1(x,t)]^r}{P^r(x,T)} \right\} \frac{\partial C_1(x,t)}{\partial x} \right)$$
(8)

$$\begin{cases} \frac{\partial I_2(x,t)}{\partial t} = \frac{\partial}{\partial x} \left[ D_I(x,T) \frac{\partial I_1(x,t)}{\partial x} \right] - k_{I,V}(x,T) [\alpha_{2I} + I_1(x,t)] [\alpha_{2V} + V_1(x,t)] - \\ -k_{I,I}(x,T) [\alpha_{2I} + I_1(x,t)]^2 \\ \frac{\partial V_2(x,t)}{\partial t} = \frac{\partial}{\partial x} \left[ D_V(x,T) \frac{\partial V_1(x,t)}{\partial x} \right] - k_{I,V}(x,T) [\alpha_{2I} + I_1(x,t)] [\alpha_{2V} + V_1(x,t)] - \\ -k_{V,V}(x,T) [\alpha_{2I} + V_1(x,t)]^2 \end{cases}$$
(9)

$$\begin{cases} \frac{\partial \Phi_{I2}(x,t)}{\partial t} = \frac{\partial}{\partial x} \left[ D_{\Phi I}(x,T) \frac{\partial \Phi_{I1}(x,t)}{\partial x} \right] + k_{I,I}(x,T) I^{2}(x,t) - k_{I}(x,T) I(x,t) \\ \frac{\partial \Phi_{V2}(x,t)}{\partial t} = \frac{\partial}{\partial x} \left[ D_{\Phi V}(x,T) \frac{\partial \Phi_{V1}(x,t)}{\partial x} \right] + k_{V,V}(x,T) V^{2}(x,t) - k_{V}(x,T) V(x,t) \end{cases}$$
(10)

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International Journal on Computational Sciences & Applications (IJCSA) Vol.4, No.2, April 2014 We obtain the second-order approximations of the required concentrations by integration of the left and right sides of the above relations. The relations could be written as

$$C_{2}(x, y, z, t) = = \frac{\partial}{\partial x} \left[ \int_{0}^{t} D_{L}(x, T) \left[ 1 + \varsigma_{1} \frac{V(x, \tau)}{V^{*}} + \varsigma_{2} \frac{V^{2}(x, \tau)}{(V^{*})^{2}} \right] \left\{ 1 + \xi \frac{[\alpha_{2c} + C_{1}(x, \tau)]^{r}}{P^{r}(x, T)} \right\} \frac{\partial}{\partial x} C_{1}(x, \tau) d\tau \right] (8a)$$

$$\begin{cases} I_{2}(x, t) = \frac{\partial}{\partial x} \left[ \int_{0}^{t} D_{I}(x, T) \frac{\partial I_{1}(x, \tau)}{\partial x} d\tau \right] - \int_{0}^{t} k_{I,I}(x, T) [\alpha_{2I} + I_{1}(x, \tau)]^{2} d\tau - \int_{0}^{t} k_{I,V}(x, T) [\alpha_{2I} + I_{1}(x, \tau)] [\alpha_{2V} + V_{1}(x, \tau)] d\tau + f_{I}(x) \\ V_{2}(x, t) = \frac{\partial}{\partial x} \left[ \int_{0}^{t} D_{V}(x, T) \frac{\partial V_{1}(x, \tau)}{\partial x} d\tau \right] - \int_{0}^{t} k_{V,V}(x, T) [\alpha_{2V} + V_{1}(x, \tau)]^{2} d\tau + \int_{0}^{t} k_{I,V}(x, T) [\alpha_{2I} + I_{1}(x, \tau)] [\alpha_{2V} + V_{1}(x, \tau)] d\tau + f_{V}(x) \end{cases}$$
(9a)

$$\begin{cases} \Phi_{I2}(x,t) = \frac{\partial}{\partial x} \begin{bmatrix} i & D_{\Phi I}(x,T) \frac{\partial \Phi_{I1}(x,\tau)}{\partial x} d\tau \end{bmatrix} + \int_{0}^{i} k_{I,I}(x,T) I^{2}(x,\tau) d\tau - \\ & -\int_{0}^{i} k_{I}(x,T) I(x,\tau) d\tau + f_{\Phi I}(x) \\ \Phi_{V2}(x,t) = \frac{\partial}{\partial x} \begin{bmatrix} i & D_{\Phi V}(x,T) \frac{\partial \Phi_{V1}(x,\tau)}{\partial x} d\tau \end{bmatrix} + \int_{0}^{i} k_{V,V}(x,T) V^{2}(x,\tau) d\tau - \\ & -\int_{0}^{i} k_{V}(x,T) V(x,\tau) d\tau + f_{\Phi V}(x) \end{cases}$$
(10a)

Average values of the second-orders approximations  $\alpha_{2\rho}$  should be determined by the standard relation [13-15,21,25,26]

$$\alpha_{2\rho} = \frac{1}{\Theta L} \int_{0}^{\Theta L} [\rho_2(x,t) - \rho_1(x,t)] dx dt.$$
(11)

Substitution of the relations (8*a*)-(10*a*) into the relation (11) gives us possibility to obtain the required relations for the values  $\alpha_{2\rho}$ 

$$\alpha_{2} = \frac{1}{L} \int_{0}^{L} f_{c}(x) dx, \qquad (12)$$

$$\begin{cases} \alpha_{2I} = \left\{ \left(1 + A_{IV01} + A_{II10} + \alpha_{2V}A_{IV00}\right)^2 - 4 \left[\alpha_{2V}A_{IV10} - A_{II20} + A_{IV11} - \frac{1}{L}\int_0^L f_I(x) dx \right] \times \\ \times A_{II00} \right\}^{\frac{1}{2}} \frac{1}{2A_{II00}} - \frac{1 + A_{IV01} + A_{II10} + \alpha_{2V}A_{IV00}}{2A_{II00}} \\ \alpha_{2V} = \frac{1}{2B_4} \sqrt{\frac{(B_3 + A)^2}{4} - 4B_4\left(y + \frac{B_3y - B_1}{A}\right)} - \frac{B_3 + A}{4B_4}, \end{cases}$$
(13)

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where 
$$A_{ubij} = \frac{1}{6L_0} \oint_{0}^{0} (\Theta - t) \int_{0}^{1} k_{u,b} (x, T) I_1^{i} (x, t) V_1^{i} (x, t) dx dt$$
,  $B_4 = A_{IV00}^2 A_{IV00}^2 - 2(A_{IV00}^2 - A_{II00} - A_{II00}$ 

$$\begin{cases} \alpha_{2\Phi_{I}} = A_{II20} - \frac{1}{\Theta L} \int_{0}^{\Theta} (\Theta - t) \int_{0}^{L} k_{I}(x, T) I(x, t) dx dt + \frac{1}{L} \int_{0}^{L} f_{\Phi I}(x) dx \\ \alpha_{2\Phi_{V}} = A_{VV20} - \frac{1}{\Theta L} \int_{0}^{\Theta} (\Theta - t) \int_{0}^{L} k_{V}(x, T) V(x, t) dx dt + \frac{1}{L} \int_{0}^{L} f_{\Phi V}(x) dx \end{cases}$$
(14)

The considered substitution gives us possibility to obtain equation for parameter  $\alpha_{2C}$ . Solution of the equation depends on value of parameter  $\gamma$ . Recently we obtain, that second-order approximation is enough good approximation to obtain main qualitative and some quantitative results. In this situation we consider second-order approximations only. Results of analytical modeling have been checked numerically.

## 3. Discussion

In this section we analyzed redistribution of dopant and radiation defects during their annealing based on distributions of their concentrations, calculated in the previous section. Figs. 3, 4 and 5 show spatial distributions of concentrations of dopant in heterostructure with one epitaxial layer (see Fig. 3) and in heterostructure with two epitaxial layers (see Figs. 4 and 5) for equal values of annealing time framework every group of curves and under condition, when value dopant diffusion coefficient in the substrate is smaller, than in doped epitaxial layer. The Figs. 4 and 5 show

International Journal on Computational Sciences & Applications (IJCSA) Vol.4, No.2, April 2014 distributions of concentration of dopant for the case, when value of dopant diffusion coefficient in external epitaxial layer is smaller and larger in comparison with value of dopant diffusion coefficient in internal epitaxial layer, respectively. One can find by consideration the figures, that presents interface between layers of heterostructure leads to increasing sharpness of *p*-*n*-junction and at the same time to increase homogeneity of distribution of concentration of dopant in doped area. Using heterostructure with two epitaxial layers gives us possibility to manufacture a bipolar transistor (see Fig. 4) or to shift from damaged during ion implantation area an implanted-junction rectifier under condition, when quantity of implanted dopant is enough large to change type of conductivity in required areas (see Fig. 5).

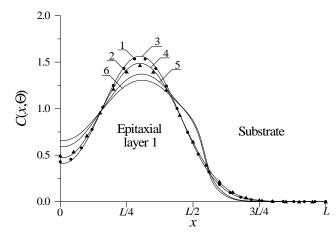


Fig. 3. Spatial distributions of implanted dopant after annealing with continuance  $\Theta = 0.0048L^2/D_0$  (curves 1, 3, 5) and  $\Theta = 0.0057L^2/D_0$  (curves 2, 4, 6). Curves 1 and 2 are experimental data for homogenous structures (see [27,28]). Curves 3 and 4 are analogous calculated distributions of concentrations of dopant. Curves 5 and 6 are calculated distributions of concentrations of dopant in heterostructure with two layers for  $D_{\text{substrate}} < D_{\text{epitaxial layer}}$  and  $\varepsilon = 0.6$ . Coordinate of interface is a = L/2

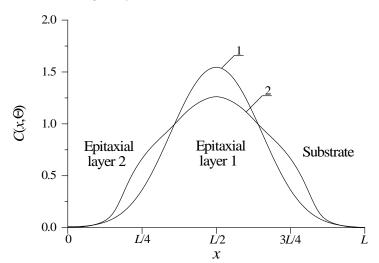


Fig. 4. Calculated spatial distributions of implanted dopant in homogenous material (curve 1) and in heterostructure with two epitaxial layers (curve 2) after annealing with continuance  $\Theta = 0.005L^2/D_0$  for  $D_{\text{epitaxial}}$  $_{\text{layer2}}=D_{\text{substrate}} < D_{\text{epitaxial layer1}}$  and  $\varepsilon = 0.6$ . Coordinates of interfaces are  $a_1 = L/4$  and  $a_2 = 3L/4$ 

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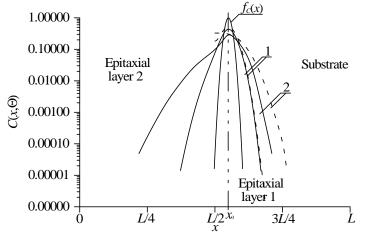


Fig. 5. Distributions of concentrations of implanted dopant in heterostructure with two epitaxial layers (solid lines) and with one epitaxial layer (dushed lines) for different values of annealing time. Increasing of number of curves corresponds to increasing of annealing time

In the ideal case implanted dopant achieves interface between layers of heterostructure during annealing. After that diffusion of dopant finishing. In this case one can obtain maximal increasing of sharpness of p-n-junction [13-15,21]. If the dopant did not achieves the interface during the annealing it is practicably to make additional annealing of dopant. In this case it is attracted an interest optimization of annealing time. We optimize annealing time framework recently introduced criterion [13-15,21]. Framework the criterion we approximate distribution of concentration of dopant by step-wise function (see Fig. 6). Farther we minimize the mean-squared error to calculate optimal value of annealing time

$$U = \frac{1}{L} \int_{0}^{L} \left[ C\left(x, \Theta\right) - \psi\left(x\right) \right] dx .$$
(15)

The Fig. 7 shows dependences of optimal annealing time on several parameters.

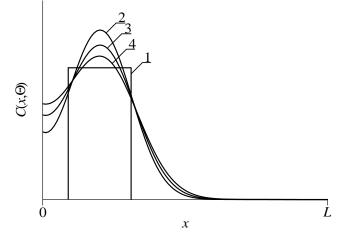


Fig.6. Spatial distributions of concentration of implanted dopant in heterostructure from Figs. 1 and 2. Curve 1 is the idealized distribution of dopant. Curves 2-4 are the real distributions of dopant for different values of annealing time. Curve 2 corresponds to minimal annealing time. Curve 3 corresponds to average annealing time. Curve 4 corresponds to maximal annealing time International Journal on Computational Sciences & Applications (IJCSA) Vol.4, No.2, April 2014

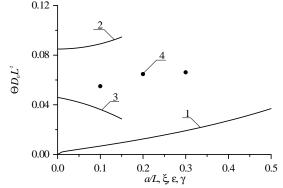


Fig.7. Dependences of dimensionless optimal annealing time for doping by ion implantation, which have been obtained by minimization of mean-squared error, on several parameters. Curve 1 is the dependence of dimensionless optimal annealing time on the relation a/L and  $\xi = \gamma = 0$  for equal to each other values of dopant diffusion coefficient in all parts of heterostructure. Curve 2 is the dependence of dimensionless optimal annealing time on value of parameter  $\varepsilon$  for a/L=1/2 and  $\xi = \gamma = 0$ . Curve 3 is the dependence of dimensionless optimal annealing time on value of parameter  $\xi$  for a/L=1/2 and  $\varepsilon = \gamma = 0$ . Curve 4 is the dependence of dimensionless optimal annealing time on value of parameter  $\gamma$  for a/L=1/2 and  $\varepsilon = \xi = 0$ 

### 4. Conclusion

In this paper we consider approaches to manufacture *p*-*n*-heterojunctions and bipolar heterotransistors. It has been shown, that using an overlayer, which has been grown over damaged area, could leads to shifting of implanted-junction rectifier from damaged area.

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