Eur. Phys. J. B **57**, 251–256 (2007)
DOI: 10.1140/epjb/e2007-00173-8

THE EUROPEAN PHYSICAL JOURNAL B

Dynamics of δ-dopant redistribution during heterostructure growth

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Received 28 November 2006/ Received in final form 6 March 2007
Published online 22 June 2007 –

Abstract. It has recently been shown that growth of a multilayer structure with one or more delta-layers at high temperature leads to spreading and asymmetrization of the dopant distribution [see, for example, E.F.J. Schubert, Vac. Sci. Technol. A. **8**, 2980 (1990), A.M. Nazmul, S. Sugahara, M. Tanaka, J. Crystal Growth **251**, 303 (2003); R.C. Newman, M.J. Ashwin, M.R. Fahy, L. Hart, S.N. Holmes, C. Roberts, X. Zhang, Phys. Rev. B **54**, 8769 (1996); E.F. Schubert, J.M. Kuo, R.F. Kopf, H.S. Luftman, L.C. Hopkins, N.J. Sauer, J. Appl. Phys. **67**, 1969 (1990); P.M. Zagwijn, J.F. van der Veen, E. Vlieg, A.H. Reader, D.J. Gravesteijn, J. Appl. Phys. **78**, 4933 (1995); W.S. Hobson, S.J. Pearton, E.F. Schubert, G. Cabaniss, Appl. Phys. Lett. **55**, 1546 (1989); *Delta Doping of Semiconductors*, edited by E.F. Schubert (Cambridge University Press, Cambridge, 1996); Yu.N. Drozdov, N.B. Baidus', B.N. Zvonkov, M.N. Drozdov, O.I. Khrykin, V.I. Shashkin, Semiconductors **37**, 194 (2003); E. Skuras, A.R. Long, B. Vogele, M.C. Holland, C.R. Stanley, E.A. Johnson, M. van der Burgt, H. Yaguchi, J. Singleton, Phys. Rev. B **59**, 10712 (1999); G. Li, C. Jagadish, Solid-State Electronics **41**, 1207 (1997)]. In this work analytical and numerical analysis of dopant dynamics in a delta-doped area of a multilayer structure has been accomplished using Fick's second law. Some reasons for asymmetrization of a delta-dopant distribution are illustrated. The spreading of a delta-layer has been estimated using example materials of a multilayer structure, a delta-layer and an overlayer.

PACS. 73.40.Kp III-V semiconductor-to-semiconductor contacts, p-n junctions, and heterojunctions – 73.40.Lq other semiconductor-to-semiconductor contacts, p-n-junctions, and heterojunctions – 66.30.-h diffusion in solids – 85.40.Ry Impurity doping, diffusion and ion implantation technology

1 Introduction

Delta-doping of solid state structures is a prospective approach for the refinement of micro- and optoelectronic devices. The technological process is widely used, for example, for refinement of parameters of Schottky diodes [11,12], heterobipolar transistors [12] and is intensively discussed in the literature (see, for example [1–12]).

The delta-doped area is a thin (with thickness approximately equal to 1 monolayer) layer, which is produced during epitaxial growth as a layer of a multilayer structure. During overgrowing of the delta-layers spreading and asymmetrization of the dopant distribution take place. Both processes lead to deviation of parameters of devices, which include itself one or more delta-layers, from estimated values.

In previous works (see, for example, [13] and the analogous works of other authors) spreading and asymmetrization of delta-dopant distribution are explained by diffusion for the simplest limiting case (for constant diffusion coefficient and symmetrical Gaussian initial distribution with negligible half-width) and segregation. The explanation has been obtained using microscopic analysis (i.e. analysis of atom migration). However, when the number of dopant atoms is large, microscopic analysis leads to lengthy calculations of dopant distribution.

Dopant dynamics depends on dynamical properties of the multilayer structure (for example, on the diffusion coefficient) and on the parameters of epitaxial growth (for example, on velocity and temperature of growth). These characteristics can be considered, when the number of the dopant atoms is large. In this case one can use Fick's laws.

The main aim of the present paper is the analysis of the influence of dynamical properties of multilayer structure and parameters of epitaxial growth on dopant redistribution during overgrowth of delta-doped areas. An accompanying aim to the previous one is development of the approach for the description of dopant redistribution taking account of the macroscopical dynamical properties of multilayer structures and parameters of epitaxial growth.

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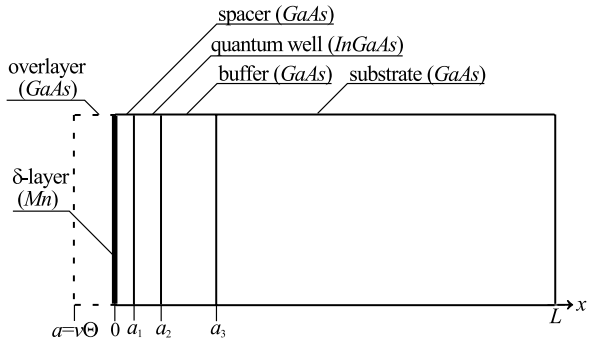

Fig. 1. Multilayer structure GaAs/InGaAs/GaAs/GaAs with δ-layer of manganese and overlayer of GaAs. Total thickness of overlayer is $a = v\Theta$, where Θ is time to complete overlayer growth, v is growth velocity.

The third aim of the paper is an estimation of the spreading of delta-dopant distribution for an example multilayer structure (see Fig. 1).

2 Method of solution

We analyzed delta-dopant redistribution to explain spreading and asymmetrization during overgrowing of a doped area. Here the spatiotemporal distribution can be described by Fick's second law [14–16]

$$p(x)\frac{\partial N(x,t)}{\partial t} = \frac{\partial}{\partial x}\left[D(x,N(x,t))\frac{\partial N(x,t)}{\partial x}\right] = -\frac{\partial J(x,t)}{\partial x}, \quad (1)$$

where $N(x,t)$ is the spatiotemporal distribution of dopant concentration, $J(x,t)$ is the spatiotemporal distribution of the dopant flow, $D(x,N(x,t))$ and $p(x)$ are the diffusion coefficient of dopant in multilayer structure and porosity of the multilayer structure respectively [14–16]. If properties of layers of the multilayer structure (see Fig. 1) differ from each other (for example, densities of the layers could differ from each other), then the diffusion coefficient and porosity of multilayer structures depends on the coordinate. Diffusion coefficient also depends on concentration. The dependence can be approximated by the power law: $D(x,N(x,t)) = D(x)\{1+\zeta[N(x,t)/P(x)]^\gamma\}$ [14]. Usually the parameter γ is an integer in the interval $1 \le \gamma \le 3$ (see, for example, [14]). $P(x)$ is the limit of solubility of the dopant in the multilayer structure.

The diffusion equation should be complemented by boundary and initial conditions. The initial distribution $N(x,0) = f(x)$ can be approximated by a Gaussian function. The half-width of the distribution at half-height is equal to the half-width of a full number of monolayers in the delta-layer. Boundary conditions near point $x = 0$ (see Fig. 1) can be written in the form: $J(-vt,t) = 0$. Usually the growth time Θ and growth temperature correspond to small diffusion length. Therefore, the second boundary condition can be written in the form $N(L,t) = 0$.

We determine a solution of the diffusion equation (1) and analyze the solution of the dopant dynamics in multilayer structure during overlayer growth. Introducing the following dimensionless coordinate, time and diffusion coefficients $\chi = (x+vt)/a$, $\vartheta = tD_0/a^2$ and $\Delta = D(x)/D_0$ leads to simplification of analysis of dopant dynamics. The introduction of the dimensionless values transforms equation (1) to the following form

$$p(\chi,\vartheta)\frac{\partial N(\chi,\vartheta)}{\partial\vartheta} = \frac{\partial}{\partial\chi}\left\{\Delta(\chi,\vartheta)\left[1+\zeta\frac{N^\gamma(\chi,\vartheta)}{P^\gamma(\chi,\vartheta)} \times\frac{\partial N(\chi,\vartheta)}{\partial\chi}\right]\right\} - \mu p(\chi,\vartheta)\frac{\partial N(\chi,\vartheta)}{\partial\chi}, \quad (2)$$

where $\mu = va/D_0$. The boundary and initial conditions for equation (1) can be written as

$$N(\chi,0) = f(\chi), J(0,\vartheta) = 0, N(\Lambda+\Xi,\vartheta) = 0,$$

where $\Lambda = L/a$, $\Xi = va\vartheta/D_0$. One can neglect Ξ in comparison with Λ for the actual values of these parameters. Therefore, the last boundary condition can be written in the form: $N(\Lambda,\vartheta) = 0$. Neglecting gives us the possibility to analyze the dopant dynamics in a moving area with length Λ. Numerical approaches give us a solution of the diffusion equation with higher precision. But the analytical solution yields a visual solution of the equation. Therefore, both approaches (analytical and numerical) have been used to analyse the dopant dynamics. We now transform equation (2) to the form

$$N(\chi,\vartheta) = \int_\Lambda^\chi \frac{1}{\Delta(v,\vartheta)}\int_0^v p(u,\vartheta)\frac{\partial N(u,\vartheta)}{\partial\vartheta}dudv + \int_\Lambda^\chi \frac{\mu}{\Delta(v,\vartheta)}\int_0^v p(u,\vartheta)\frac{\partial N(u,\vartheta)}{\partial u}dudv - \xi\int_\Lambda^\chi\left[\frac{N(v,\vartheta)}{P(v,\vartheta)}\right]dv. \quad (3)$$

We use the method of averaging of function corrections [17] for the solution of equation (3). Substitution of the the average value of dopant concentration

$$\alpha_1 = \frac{1}{\Theta\Lambda}\int_0^\Theta\int_0^\Lambda N_1(\chi,\vartheta)d\chi d\vartheta$$

and/or the average value of the partial derivatives of dopant concentration

$$\beta_1 = \frac{1}{\Theta\Lambda}\int_0^\Theta\int_0^\Lambda \frac{\partial N_1(\chi,\vartheta)}{\partial\chi}d\chi d\vartheta,$$

$$\omega_1 = \frac{1}{\Theta\Lambda}\int_0^\Theta\int_0^\Lambda \frac{\partial N_1(\chi,\vartheta)}{\partial\vartheta}d\chi d\vartheta$$

instead of dopant concentration $N(\chi,\vartheta)$ and/or partial derivatives of dopant concentration gives us the possibility to calculate the first-order approximation to the dopant concentration $N_1(\chi,\vartheta)$ in order to use the method of averaging of function correction in the classical form. Let us substitute the solution of the diffusion equation with the average value of diffusion coefficient D_0 and porosity p_0 instead of average value of dopant concentration in order to calculate the first-order approximation of dopant concentration. This substitution leads to accelerated convergence of the method of averaging of function corrections. The solution of the diffusion equation with averaged parameters D_0 and p_0 can be written in the form

$$N(\chi,\vartheta)=2\sum_{n=0}^{\infty}F_{n+0.5}c_{n+0.5}(\chi)e_{n+0.5}(\vartheta), \qquad (4)$$

where $c_n(\chi)=\cos(\pi n\chi)$, $F_n=\int\limits_0^{\Lambda}f(v)c_n(v)dv$, $e_n(\vartheta)=\exp(-\pi^2n^2\vartheta)$. The first-order approximation to dopant concentration $N_1(\chi,\vartheta)$, which corresponds to relation (4), can be written in the form

$$\begin{aligned}N_1(\chi,\vartheta)&=2^{\gamma+1}\pi\xi\sum_{n=0}^{\infty}F_{n+0.5}c_{n+0.5}(\chi)e_{n+0.5}(\vartheta)\\&\times\int\limits_0^{\chi}\left[\sum_{m=0}^{\infty}F_{m+0.5}c_{m+0.5}(v)e_{m+0.5}(\vartheta)\right]^{\gamma}\frac{s_{m+0.5}(v)}{P^{\gamma}(v,\vartheta)}\\&\times\frac{p(v,\vartheta)}{\Delta(v,\vartheta)}dv-2\pi^2\sum_{n=0}^{\infty}F_{n+0.5}e_{n+0.5}(\vartheta)\\&\times\int\limits_0^{\chi}\frac{Gc_n(v,\vartheta)}{\Delta(v,\vartheta)}dv-2\pi\mu\sum_{n=0}^{\infty}F_{n+0.5}e_{n+0.5}(\vartheta)\\&\times\int\limits_0^{\chi}\frac{Gc_n(v,\vartheta)}{\Delta(v,\vartheta)}dv, \qquad (5)\end{aligned}$$

where $s_n(\chi)=\sin(\pi n\chi)$, $Gy_n(\chi,\vartheta)=\int\limits_0^{\chi}p(v,\vartheta)y_n(v)dv$. The second-order approximation of dopant concentration can be calculated by standard substitution of the sum $\alpha_2+N_1(\chi,\vartheta)$ instead of dopant concentration $N(\chi,\vartheta)$ in equation (2) [17]. The substitution leads to the following relation

$$\begin{aligned}N_2(\chi,\vartheta)&=\int\limits_0^{\chi}\frac{1}{\Delta(v,\vartheta)}\int\limits_0^{v}p(u,\vartheta)\frac{\partial N_1(u,\vartheta)}{\partial\vartheta}dudv\\&+\mu\int\limits_0^{\chi}\frac{1}{\Delta(v,\vartheta)}\int\limits_0^{v}p(u,\vartheta)\frac{\partial N_1(u,\vartheta)}{\partial u}dudv\\&-\xi\int\limits_0^{\chi}\left[\frac{\alpha_2+N_1(v,\vartheta)}{P(v)}\right]^{\gamma}\frac{\partial N_1(v,\vartheta)}{\partial v}dv. \qquad (6)\end{aligned}$$

The parameter α_2 can be determined from the following expression [17]

$$\alpha_2=\frac{M_2-M_1}{\Theta\Lambda}, \qquad (7)$$

where $M_i=\int\limits_0^{\Theta}\int\limits_0^{\Lambda}N_i(\chi,\vartheta)d\chi d\vartheta$. Substituting (5) and (6) into (7) yields

$$\begin{aligned}\alpha_2(\gamma=1)&=\frac{\xi\Omega_{11}-\Psi_{\vartheta}-\mu\Psi_u}{\Theta\Lambda-\xi\Omega_{11}},\\\alpha_2(\gamma=2)&=-\frac{2\xi\Omega_{12}-\Theta\Lambda}{2\xi\Omega_{12}}\\&+\left[\frac{2\xi\Omega_{12}-\Theta\Lambda}{2\xi\Omega_{02}}-\frac{4}{2\xi\Omega_{01}}\left(\xi\Omega_{22}-\Psi_{\vartheta}-\mu\Psi_u-M_1\right)^2\right]^{\frac{1}{2}},\\\alpha_2(\gamma=3)&=\left[\left(\frac{p^3}{27}+\frac{q^2}{4}\right)^{\frac{1}{2}}-\frac{q}{2}\right]^{\frac{1}{3}}\\&-\left[\left(\frac{p^3}{27}+\frac{q^2}{4}\right)^{\frac{1}{2}}+\frac{q}{2}\right]^{\frac{1}{3}}+\frac{3\Omega_{13}}{\Omega_{03}},\end{aligned}$$

where $q=\frac{\xi\Omega_{33}-M_1-\Psi_{\vartheta}-\mu\Psi_u}{\xi\Omega_{03}}-\Omega_{13}\frac{3\xi\Omega_{23}-\Theta\Lambda}{\xi\Omega_{03}^2}+\frac{3\Omega_{13}^3}{\Omega_{03}^3}$, $\Omega_{ij}=\int\limits_0^{\Theta}\int\limits_0^{\Lambda}\frac{vN_1^i(v,\vartheta)}{P^j(v,\vartheta)}\frac{\partial N_1(v,\vartheta)}{\partial v}dvd\vartheta, q=\frac{3\xi\Omega_{23}-\Theta\Lambda}{\Omega_{03}}-\frac{3\Omega_{13}^2}{\Omega_{03}^2}$, $\Psi_{\lambda}=\int\limits_0^{\Theta}\int\limits_0^{\Lambda}\frac{v}{\Delta(v,\vartheta)}\int\limits_0^{v}p(u,\vartheta)\frac{\partial N_1(u,\vartheta)}{\partial\lambda}dudvd\vartheta$.

It can be shown that consideration of the second-order approximation of dopant concentration, obtained by averaging of function corrections, allows analysis of dopant dynamics during overlayer growth without lengthy calculations.

Further let us analyze the dopant dynamics for different regimes of epitaxial overlayer growth using the approximation of dopant concentration. Good behavior of the analytical solution of equation (1) in comparison with the numerical one gives us the possibility to determine some dependencies of dopant concentration on different parameters and to estimate approximately the spreading of the delta-layer. Using numerical approaches leads to increased precision of the spatiotemporal distribution of dopant concentration and estimation of delta-layer spreading.

3 Discussion

First of all let us consider the multilayer structure growth regime, when a pause between finishing the delta-layer growth and starting the overlayer growth takes a place. The pause leads to dopant diffusion into the spacer during the pause. Therefore, dopant distribution in the delta-doped area will be initially asymmetrical. The initial asymmetrization is, probably, the first reason for asymmetrization of dopant distribution and could be accounted here by considering an asymmetrical initial distribution.

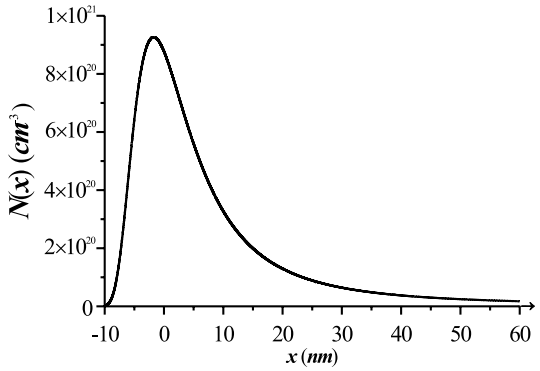

Fig. 2. Dopant distribution in a δ-doped area taking account the pause between finishing δ-layer growth and beginning overlayer growth.

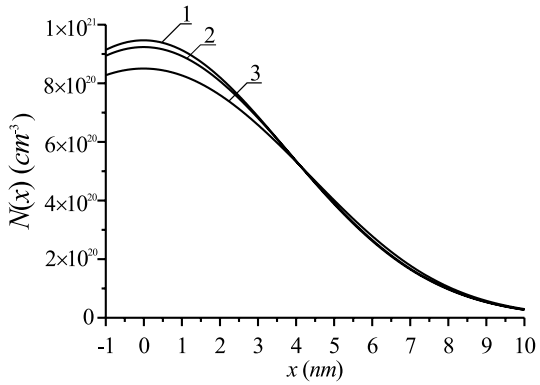

Fig. 3. Spatial distribution of manganese concentration for the regime of small value of growth velocity or short-time growth with large value of the growth velocity of overlayer for equal dynamic properties of layers of the multilayer structure. Growth temperature is equal to 300 °C, 400 °C and 450 °C (curves 1, 2 and 3 respectively).

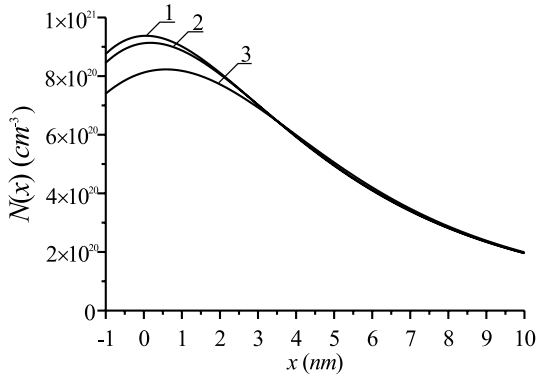

Fig. 4. Spatial distribution of manganese concentration for the regime of small value of growth velocity or short-time growth with large value of the growth velocity of the overlayer with differing dynamic properties of layers of the multilayer structure. Growth temperature is equal to 300 °C, 400 °C and 450 °C (curves 1, 2 and 3 respectively).

An example of spatial distribution of dopant with an asymmetrical initial distribution is presented in Figure 2. However, the asymmetrization indicates delta-layer degradation. Therefore, the pause between finishing the delta-layer growth and starting of overlayer growth should be decreased. Let us consider further the limiting case of the short pause regime.

The alternative classification of overgrowth regimes could be considered with account of velocity and time of overgrowth. The first regime of the second classification is a regime with small value of the growth velocity or short-time growth with large value of the growth velocity. In that case dopant concentration $N(0, \vartheta)$ is always nonzero. Maximal growth time in that case could be estimated from the following expression: $\sqrt{D_0\Theta/p_0} > v\Theta$. The left side of the expression is an estimation of the diffusion length of the dopant in the overlayer after finishing the layer growth. The right side of the last relation is the thickness of the overlayer, when the growth time is equal to Θ. The inequality could be transformed to the form: $\Theta < D_0/p_0v^2$. Spatial distribution of dopant concentration in the multilayer structure (Fig. 1) for the considered case is illustrated by Figure 3 (for the case, when dynamical properties of the layers are equal to each other) and 4 (for the case, when dynamical properties of the overlayer and spacer differ from each other). Temperature dependence of diffusion coefficient and limit of solubility of manganese in gallium arsenide are presented, for example, in [18] and in references of reference [19], respectively. We consider such time, velocity and temperature of overlayer growth, that correspond to zero concentration of the dopant in the quantum well.

The second regime of overlayer growth is regime of long-time growth with large value of the growth velocity. Here the dopant concentration $N(0, \vartheta)$ is always zero. Minimal growth time for consideration of the case could be estimated from the following expression: $\Theta > D_0/p_0v^2$. Spatial distribution of dopant concentration for the case is illustrated in Figures 5 (if the dynamical properties of the multilayer layers are similar) and 6 (if the dynamical properties of overlayer and spacer differ from each other). Pair comparison of Figures 3 and 4, 5 and 6 illustrate, that the difference between dynamical properties of overlayer and spacer leads to asymmetrization of spatial distribution of dopant in the delta-doped area. The asymmetrisation of dopant distribution due to the difference between dynamical properties of the multilayer structure layers (see Fig. 1) is, probably, the second route to asymmetrisation of dopant distribution during overgrowth.

The analysis of dopant redistribution leads to the following conclusion: to decrease asymmetrization of delta-dopant distribution the inequality $D_1/p_1 > D_2/p_2$ should be achieved. Here D_1 and p_1 are the parameters of the overlayer, D_2 and p_2 are parameters of the spacer.

Spatial distribution of dopant concentration depends on the type of nonlinearity of multilayer structure materials. Dependencies of the dopant distribution on parameters γ and ζ are illustrated in Figures 7 and 8. One can see from the figures, that increasing the parameters γ and ζ leads to increasing spreading of the delta-layer. Figure 9 illustrates a comparison of quantities calculated in this

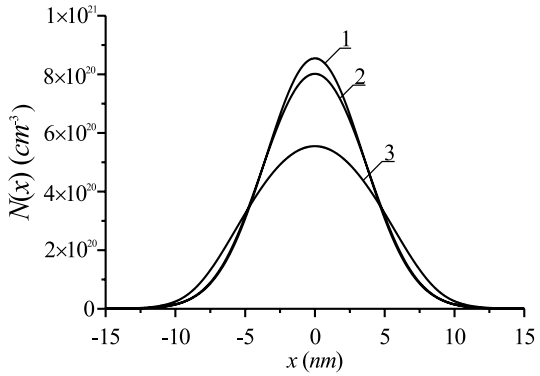

Fig. 5. Spatial distribution of manganese concentration, for the regime of long-time growth of the overlayer with large growth velocity and equivalent to each other dynamic properties for the layers of the multilayer structure. Growth temperature is 300 °C, 450 °C and 500 °C (curves 1, 2 and 3 respectively).

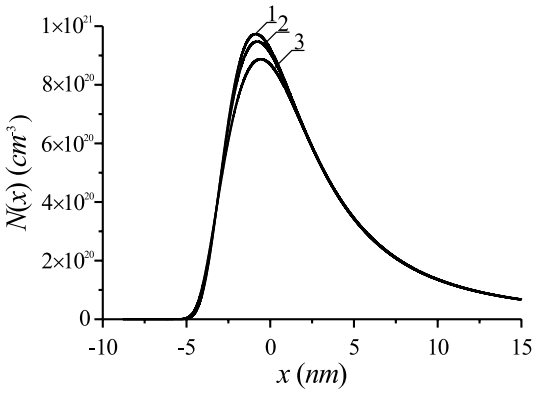

Fig. 6. Spatial distribution of manganese concentration for the regime of long-time growth of overlayer with large growth velocity for with differing dynamics properties of layers in the multilayer structure. Growth temperature is 300 °C, 450 °C and 500 °C (curves 1, 2 and 3 respectively).

paper and measured and presented (Ref. [2]) spatial distributions of manganese concentration in multilayer structure GaAs /InGaAs/GaAs/GaAs for different growth temperature.

Further let us estimate the spreading of the delta-layer. For the estimation we used two criteria. The first gives us an estimation of the delta-layer spreading as a variation of the half-width of the delta-layer at the half-height of the maximal value of the dopant concentration. The second criterion is known as the "equiareal rectangle". The second criterion is considered in detail, for example, in references [20–23]. Both criteria lead to approximately equal results. Dopant diffusion in the quantum well is usually unwanted. Therefore, first of all we considered right-sided spreading of the delta-layer. The dimensionless spreading of the delta-layer $\eta = d/b$ is presented in Figures 10 and 11 as functions of growth temperature and thickness of overlayer, where d is real spreading, b is half-thickness of initial distribution of dopant. One can see from the figures that

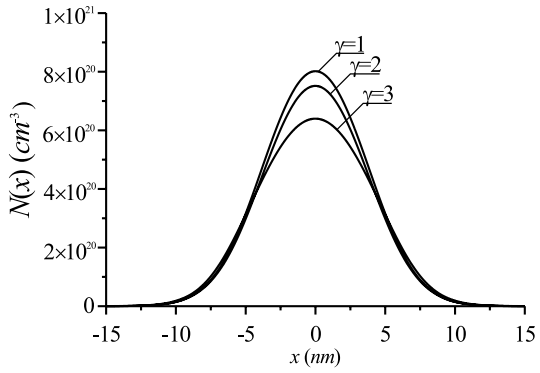

Fig. 7. Dependence of spatial distribution of manganese concentration on parameter γ. Growth temperature is 450 °C.

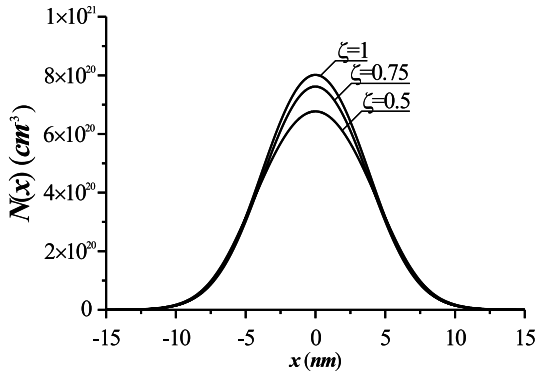

Fig. 8. Dependence of spatial distribution of manganese concentration on parameter ζ. Growth temperature is 450 °C.

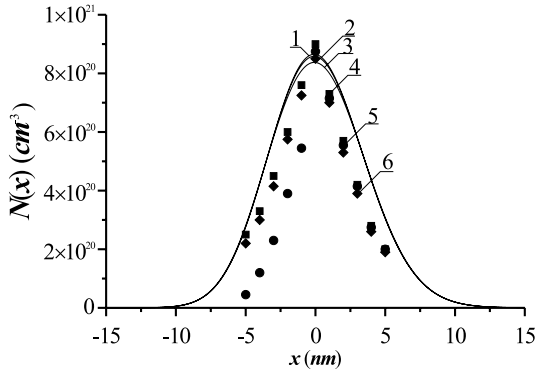

Fig. 9. Comparison of calculations in this paper (solid lines) and measured (Ref. [2]) spatial distribution of manganese concentration. Growth temperature is 220 °C (curves 1 and 4), 300 °C (curves 2 and 5) and 400 °C (curves 3 and 6).

increasing both parameters lead to a linear increase of the spreading.

4 Conclusions

In the present paper the analysis of delta-dopant distribution spreading and asymmetrization in a multilayer structure during dopant overgrowth has been accomplished using Fick's second law. The law allows consideration

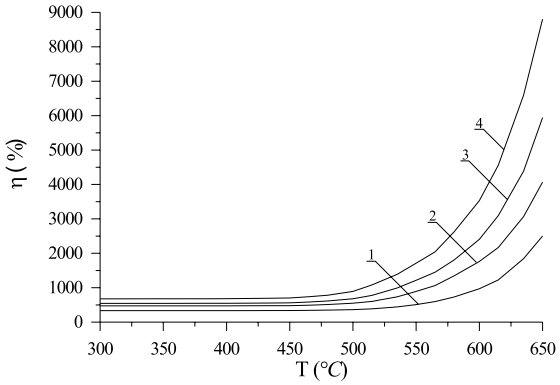

Fig. 10. Dependence of dimensionless spreading of δ-layer on growth temperature for different values of overlayer thicknesses. Curve 1 corresponds to 50 nm, curve 2 corresponds to 100 nm, curve 3 corresponds to 150 nm, curve 4 corresponds to 200 nm.

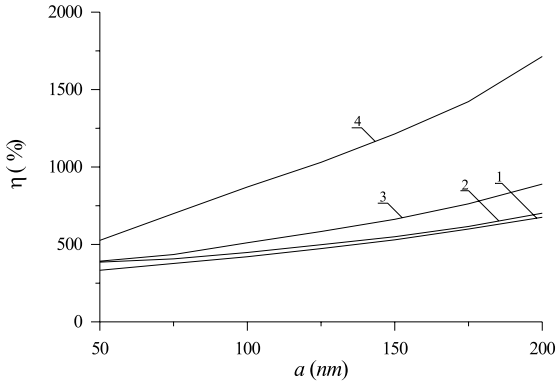

Fig. 11. Dependence of dimensionless spreading of δ-layer on thickness of overlayer for growth temperatures of 300 °C (curve 1), 400 °C (curve 2), 450 °C (curve 3) and 500 °C (curve 4).

of dopant diffusion during overgrowth. This leads to a complete explanation of the spreading and asymmetrization of dopant distribution without considering any additional processes, such as segregation. Analysis of dopant redistribution during overgrowth gives several conditions for decrease of asymmetrization of delta-dopant distribution. Spreading of a delta-layer in a multilayer structure during growth of an overlayer has been estimated. As an example of materials we considered a delta-layer of manganese (1.7 monolayer), multilayer structure GaAs/InGaAs/GaAs/GaAs and overlayer of GaAs (see Fig. 1). The estimation of spreading has been analyzed as a function of the growth temperature and growth time.

This work has been supported by Contract (project 02.442.11.7342).

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