International Journal of Physics and Mathematics
www.physicsjournal.net
Online ISSN: 2664-8644; Print ISSN: 2664-8636
Received: 03-05-2019; Accepted: 05-06-2019; Published: 12-06-2019
Volume 1; Issue 2; 2019; Page No. 29-33

Changing of properties of epitaxial layers by choosing of temperature field during growth

EL Pankratov[1]
[1] Nizhny Novgorod State University, 23 Gagarin Avenue, Nizhny Novgorod, Russia
[1] Nizhny Novgorod State Technical University, 24 Minin Street, Nizhny Novgorod, Russia

Abstract
In this paper, we analyze the influence of the temperature of growth of epitaxial layers during their growth. Conditions are formulated under which the homogeneity of the properties of the epitaxial layers increases. An analytical approach for the analysis of mass and heat transfer is proposed, allowing at the same time to take into account changes in the parameters of processes both in space and in time, as well as nonlinearity of these processes.

Keywords: prognosis of epitaxial growth; changing of properties of epitaxial layers; analytical approach for analysis

Introduction

The development of solid-state electronics and the widespread using of heterostructures for the manufacturing of electronic devices leads to the need to improvement of properties of the materials used. For the manufacturing of heterostructures one can use different methods: molecular beam epitaxy, epitaxy from the gas phase, magnetron sputtering. A large number of experimental studies are devoted to the manufacture and use of heterostructures due to their widely using [1, 10]. At the same time, a relatively small number of papers [10] are devoted to predicting epitaxy processes. This paper considers a two-layer structure consisting of a substrate and a growing epitaxial layer (see Fig. 1). The main aim of the paper is analysis of changes of temperature of growth of the epitaxial layer on its properties. An accompanying aim of the paper is development of analytical approach for analyzing of mass and heat transfer, which simultaneously takes into account changes in the parameters of processes both in space and in time, as well as the nonlinearity of these processes.

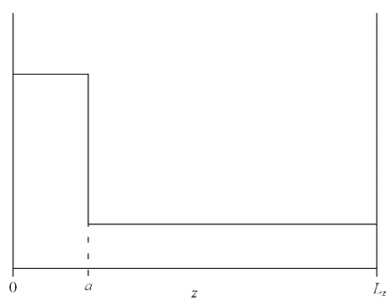

Fig 1: Heterostructure, which consist of a substrate and an epitaxial layer

Method of solution

To solve this aim, we determine the concentration of the growth component $C(x,t)$. The required concentration was determined by solving the following boundary value problem

$$\frac{\partial C(x,t)}{\partial t} = \frac{\partial}{\partial x}\left[D_C \frac{\partial C(x,t)}{\partial x}\right] \tag{1}$$

$$\left.\frac{\partial C(x,t)}{\partial x}\right|_{x=-vt} = 0,\ \left.\frac{\partial C(x,t)}{\partial x}\right|_{x=L} = 0,\ C(x,0)=f(x). \tag{2}$$

It should be noted that the material of the epitaxial layer does not reach the boundary $x=L$. For this reason, we can assume that $C(L,t)=0$. In relations (1) and (2), the following notation is introduced: T is the annealing temperature, D_C is the diffusion coefficient, v is the speed of epitaxial growth. The value of the diffusion coefficient is determined by the properties of the materials in the layers of the heterostructure, the rate of heating and cooling of the heterostructure (in accordance with the Arrhenius law). The dependences of the diffusion coefficient on the parameters can be approximated by the following relation [11, 13]

$$D_C = D_L(x,T)\left[1+\xi\frac{C^{\gamma}(x,t)}{P^{\gamma}(x,T)}\right]. \tag{3}$$

Here $D_L(x, T)$ is the dependence of the diffusion coefficient on the coordinate (due to dependence of properties of the heterostructure on coordinate) and temperature (according to the Arrhenius law); $P(x, T)$ is the limit of solubility of material of epitaxial layer (if we consider only epitaxial layer than $\xi=0$); determined by the properties of the material, the parameter γ can take integer values in the interval $\gamma\in$ [1, 3, 12]. The concentration dependence of the diffusion coefficient is discussed in detail in [12]. Next, we replace variables x and t and the diffusion coefficient $D_L(x)$ to the dimensionless variables χ and ϑ and the normalized diffusion coefficient $\Delta(x)$ introduced by the following relations $x\to\chi=(x+v\,t)/a$, $t\to\vartheta=tD_0/a^2$ and $\Delta=D_L(x)/D_0$, where D_0 is the average value of the diffusion coefficient. Given such a replacement, the diffusion equation takes the form

$$\frac{\partial C(\chi,\vartheta)}{\partial\vartheta}=\frac{\partial}{\partial\chi}\left\{\Delta(\chi,\vartheta)\left[1+\varsigma\frac{C^{\gamma}(\chi,\vartheta)}{P^{\gamma}(\chi,\vartheta)}\right]\frac{\partial C(\chi,\vartheta)}{\partial\chi}\right\}-\mu\frac{\partial C(\chi,\vartheta)}{\partial\chi}. \tag{4}$$

Here $\mu=va/D_0$. The boundary and initial conditions in the new variables are written in the following form: $C(\chi, 0)=f(\chi)$, $J(0,\vartheta)=0$, $C(X+\Xi,\vartheta)=0$, where $X=L/a$, $\Xi=va\vartheta/D_0$. In the vicinity of the boundary $x=L$ (i.e., $\chi=X+\Xi$) of the considered structure, the epitaxial layer - substrate (Fig. 1), the term Ξ can be neglected as compared to the term X. Such an approximation allows us to write the last boundary condition in a simplified form: $C(X,\vartheta)=0$ and analyze the dynamics of material of epitaxial layer in a moving region of length X. To estimate the spatio-temporal distribution of material of epitaxial layer, analytical methods are of primary interest because of their greater visibility compared to numerical methods. The analytical estimate of the function $C(\chi,\vartheta)$ is carried out by solving the equivalent equation (4) of the integro-differential equation of the following form

$$C(\chi,\vartheta)=\int_0^{\chi}\frac{1}{\Delta(v,\vartheta)}\int_0^{v}\frac{\partial C(u,\vartheta)}{\partial\vartheta}\,d\,u\,d\,v+\int_0^{\chi}\frac{\mu}{\Delta(v,\vartheta)}\int_0^{v}\frac{\partial C(u,\vartheta)}{\partial u}\,d\,u\,d\,v-\,-\varsigma\int_0^{\chi}\frac{C^{\gamma}(v,\vartheta)}{P^{\gamma}(v,\vartheta)}\frac{\partial C(v,\vartheta)}{\partial v}\,d\,v. \tag{5}$$

The solution of this equation will be sought by averaging functional corrections [14]. In the first approximation by the averaging method, the function $C(\chi,\vartheta)$ and its derivatives are replaced by their constant components on the right side of equation (3): $C(\chi,\vartheta)\to\alpha_1$, $\partial C(\chi,\vartheta)/\partial\vartheta\to\beta_1$ and $\partial C(\chi,\vartheta)/\partial\chi\to\omega_1$. Further, the resulting solution is specified. However, replacing the function $C(\chi,\vartheta)$ with a more accurate approximation in the right side of Eq. (5) allows us to speed up the convergence of the algorithm for estimating the solution of Eq. (5). As a more accurate approximation, we use the solution of the diffusion equation in the simplest case of a constant diffusion coefficient and fixed in time boundaries of the structure of the epitaxial layer - substrate. It can be shown (see, for example [15], that the constant component of the diffusion coefficient D_0 is often most successful when choosing a constant approximation of changes in the diffusion coefficient. The solution of the diffusion equation with a constant diffusion coefficient can be obtained by standard methods (see, for example [16, 17], and written in the following form

$$\tilde{C}(\chi,\vartheta)=2\sum_{n=0}^{\infty}\int_0^{X}f(\chi)\cos[\pi(n+0.5)\chi]\,d\,\chi\cos[\pi(n+0.5)\chi]\,\exp\left[-\pi^2(n+0.5)^2\vartheta\right]. \tag{6}$$

Substituting of relation (6) into Eq. (5) gives a possibility to obtain the first-order approximation of the concentration of the material of the epitaxial layer

$$C_1(\chi,\vartheta)=\pi\varsigma\sum_{n=0}^{\infty}\exp\left[-\pi^2(n+0.5)^2\vartheta\right]\int_0^{X}f(\chi)\cos[\pi(n+0.5)\chi]\,d\,\chi\int_0^{\chi}\frac{\sin[\pi(n+0.5)v]}{\Delta(v,\vartheta)P^{\gamma}(v,\vartheta)}\times$$

$$\times\left[\sum_{m=0}^{\infty}\int_0^{X}f(\chi)\cos[\pi(m+0.5)\chi]d\,\chi\cos[\pi(m+0.5)\chi]\exp\left[-\pi^2(m+0.5)^2\vartheta\right]\right]^{\gamma}d\,v(n+0.5)\times$$

$$\times 2^{\gamma+1}-2\pi\sum_{n=0}^{\infty}\int_0^{X} f(\chi)\cos[\pi(n+0.5)\chi]\,d\chi\,\exp\left[-\pi^2(n+0.5)^2\vartheta\right]\int_0^{\chi}\frac{\sin[\pi(n+0.5)v]}{\Delta(v,\vartheta)}dv\times$$

$$\times(n+0.5)+2\mu\sum_{n=0}^{\infty}\int_0^{\chi}\Delta^{-1}(v,\vartheta)\cos[\pi(n+0.5)v]\,dv\int_0^{X} f(\chi)\cos[\pi(n+0.5)\chi]\,d\chi\times$$

$$\times\exp\left[-\pi^2(n+0.5)^2\vartheta\right]. \qquad (7)$$

The second-order approximation of the function $C(\chi,\vartheta)$ can be obtained by the standard (see, for example [14], replacement on the right side of equation (4), i.e. $C(\chi,\vartheta)\to\alpha_2+C_1(\chi,\vartheta)$. The replacement leads to the following result

$$C_2(\chi,\vartheta)=\int_0^{\chi}\frac{1}{\Delta(\chi,\vartheta)}\int_0^{v}\frac{\partial C_1(u,\vartheta)}{\partial\vartheta}du\,dv+\mu\int_0^{\chi}\frac{C_1(v,\vartheta)}{\Delta(v,\vartheta)}dv-\;-\varsigma\int_0^{\chi}\left[\frac{\alpha_2+C_1(v,\vartheta)}{P(v,\vartheta)}\right]^{\gamma}\frac{\partial C_1(v,\vartheta)}{\partial v}dv\cdot \qquad (8)$$

Parameter α_2 could be determine by the following relation [14]

$$\alpha_2=\frac{1}{\Theta X}\int_0^{\Theta}\int_0^{X}\left[C_2(\chi,\vartheta)-C_1(\chi,\vartheta)\right]d\chi\,d\vartheta. \qquad (9)$$

Substitution of relations (7) and (8) into (9) leads to the following result

$$\alpha_2(\gamma=1)=\left[\varsigma\int_0^{\Theta}\int_0^{X}\chi\frac{C_1(\chi,\vartheta)}{P(\chi,\vartheta)}\frac{\partial C_1(\chi,\vartheta)}{\partial\chi}d\chi\,d\vartheta-\int_0^{\Theta}\int_0^{X}\int_0^{\chi}\frac{\partial C_1(u,\vartheta)}{\partial\vartheta}du\frac{\chi\,d\chi\,d\vartheta}{\Delta(\chi,\vartheta)}-\right.$$

$$\left.-\int_0^{\Theta}\int_0^{X}C_1(\chi,\vartheta)d\chi\,d\vartheta-\mu\int_0^{\Theta}\int_0^{X}C_1(\chi,\vartheta)\frac{\chi\,d\chi\,d\vartheta}{\Delta(\chi,\vartheta)}\right]\left[\Theta X-\varsigma\int_0^{\Theta}\int_0^{X}\chi\frac{C_1(\chi,\vartheta)}{P(\chi,\vartheta)}\frac{\partial C_1(\chi,\vartheta)}{\partial\chi}d\chi\,d\vartheta\right]^{-1},$$

$$\alpha_2(\gamma=2)=-\frac{2\varsigma\int_0^{\Theta}\int_0^{X}\chi\frac{C_1(\chi,\vartheta)}{P^2(\chi,\vartheta)}\frac{\partial C_1(\chi,\vartheta)}{\partial\chi}d\chi\,d\vartheta-\Theta X}{2\varsigma\int_0^{\Theta}\int_0^{X}\chi\frac{C_1(\chi,\vartheta)}{P^2(\chi,\vartheta)}\frac{\partial C_1(\chi,\vartheta)}{\partial\chi}d\chi\,d\vartheta}+$$

$$+\left\{\frac{2\varsigma\int_0^{\Theta}\int_0^{X}\chi\frac{C_1(\chi,\vartheta)}{P^2(\chi,\vartheta)}\frac{\partial C_1(\chi,\vartheta)}{\partial\chi}d\chi\,d\vartheta-\Theta X}{2\varsigma\int_0^{\Theta}\int_0^{X}\frac{\partial C_1(\chi,\vartheta)}{\partial\chi}\frac{\chi\,d\chi\,d\vartheta}{P^2(\chi,\vartheta)}}-\frac{4}{\varsigma\int_0^{\Theta}\int_0^{X}\frac{\partial C_1(\chi,\vartheta)}{\partial\chi}\frac{\chi\,d\chi\,d\vartheta}{P^2(\chi,\vartheta)}}\times\right.$$

$$\times\left[\varsigma\int_0^{\Theta}\int_0^{X}\chi\frac{C_1^2(\chi,\vartheta)}{P^2(\chi,\vartheta)}\frac{\partial C_1(\chi,\vartheta)}{\partial\chi}d\chi\,d\vartheta-\int_0^{\Theta}\int_0^{X}\frac{\chi}{\Delta(\chi,\vartheta)}\int_0^{\chi}\frac{\partial C_1(u,\vartheta)}{\partial\vartheta}du\,d\chi\,d\vartheta-\right.$$

$$\left.\left.-\mu\int_0^{\Theta}\int_0^{X}\chi\frac{C_1(\chi,\vartheta)}{\Delta(\chi,\vartheta)}d\chi\,d\vartheta-\int_0^{\Theta}\int_0^{X}C_1(\chi,\vartheta)d\chi\,d\vartheta\right]^2\right\}^{\frac{1}{2}}$$

$$\alpha_2(\gamma=3)=\sqrt[3]{\sqrt{\frac{p^3}{27}+\frac{q^2}{4}}-\frac{q}{2}}-\sqrt[3]{\sqrt{\frac{p^3}{27}+\frac{q^2}{4}}+\frac{q}{2}}+3\frac{\int_0^\Theta\int_0^X \chi\frac{C_1(\chi,\vartheta)}{P^3(\chi,\vartheta)}\frac{\partial C_1(\chi,\vartheta)}{\partial\chi}d\chi\, d\vartheta}{\int_0^\Theta\int_0^X \chi\frac{\partial C_1(\chi,\vartheta)}{\partial\chi}\frac{d\chi\, d\vartheta}{P^3(\chi,\vartheta)}}.$$

Here $p=\left\{\int_0^\Theta\int_0^X \frac{\partial C_1(\chi,\vartheta)}{\partial\chi}\frac{\chi\, d\chi\, d\vartheta}{P^3(\chi,\vartheta)}\left[3\varsigma\int_0^\Theta\int_0^X \chi\frac{C_1^2(\chi,\vartheta)}{P^3(\chi,\vartheta)}\frac{\partial C_1(\chi,\vartheta)}{\partial\chi}d\chi\, d\vartheta-\Theta X\right]-3\left[\int_0^\Theta\int_0^X \chi\frac{C_1(\chi,\vartheta)}{P^3(\chi,\vartheta)}\times\right.\right.$

$$\left.\left.\times\frac{\partial C_1(\chi,\vartheta)}{\partial\chi}d\chi\, d\vartheta\right]^2\right\}\left[\int_0^\Theta\int_0^X \frac{\partial C_1(\chi,\vartheta)}{\partial\chi}\frac{\chi\, d\chi\, d\vartheta}{P^3(\chi,\vartheta)}\right]^2,\ q=2\left[\int_0^\Theta\int_0^X \chi\frac{C_1(\chi,\vartheta)}{P^3(\chi,\vartheta)}\frac{\partial C_1(\chi,\vartheta)}{\partial\chi}d\chi\, d\vartheta\right]^3\times$$

$$\times\left[\int_0^\Theta\int_0^X \frac{\partial C_1(\chi,\vartheta)}{\partial\chi}\frac{\chi\, d\chi\, d\vartheta}{P^3(\chi,\vartheta)}\right]^{-3}-\left[3\int_0^\Theta\int_0^X \chi\frac{C_1^2(\chi,\vartheta)}{P^3(\chi,\vartheta)}\frac{\partial C_1(\chi,\vartheta)}{\partial\chi}d\chi\, d\vartheta-\frac{\Theta X}{\varsigma}\right]\int_0^\Theta\int_0^X \chi\frac{C_1(\chi,\vartheta)}{P^3(\chi,\vartheta)}\times$$

$$\times\frac{\partial C_1(\chi,\vartheta)}{\partial\chi}d\chi\, d\vartheta\left[\int_0^\Theta\int_0^X \frac{\partial C_1(\chi,\vartheta)}{\partial\chi}\frac{\chi\, d\chi\, d\vartheta}{P^3(\chi,\vartheta)}\right]^2+\left[\varsigma\int_0^\Theta\int_0^X \chi\frac{C_1^3(\chi,\vartheta)}{P^3(\chi,\vartheta)}\frac{\partial C_1(\chi,\vartheta)}{\partial\chi}d\chi\, d\vartheta-\right.$$

$$\left.-\int_0^\Theta\int_0^X\int_0^\chi \frac{\partial C_1(u,\vartheta)}{\partial\vartheta}du\frac{\chi\, d\chi\, d\vartheta}{\Delta(\chi,\vartheta)}-\int_0^\Theta\int_0^X C_1(\chi,\vartheta)d\chi\, d\vartheta-\mu\int_0^\Theta\int_0^X\int_0^\chi \frac{\partial C_1(u,\vartheta)}{\partial u}du\frac{\chi\, d\chi\, d\vartheta}{\Delta(\chi,\vartheta)}\right]\times$$

$$\times\left[\varsigma\int_0^\Theta\int_0^X \frac{\partial C_1(\chi,\vartheta)}{\partial\chi}\frac{\chi\, d\chi\, d\vartheta}{P^3(\chi,\vartheta)}\right]^{-1}.$$

The second-order approximation of the material concentration gives a possibility to obtain the main physical conclusions from the analysis of the spatio-temporal distribution of the considered concentration in different growth modes of the heterostructure. If necessary, approximations of the third, fourth, etc. orders could be obtained by analogous way with the second order approximation. In order to check the results obtained, numerical methods were also used. But numerical methods are less visual than analytical ones.

Discussion

In this section, we will analyze the spatio-temporal distribution of the concentration of the material of the epitaxial layer in the considered heterostructure. An example of spatial distributions of the considered material we present comparison of these distribution on Fig.2. This figure shows an increasing of homogeneity of concentration of the material of the epitaxial layer with increasing of growth temperature. At the same time, the sharpness of the interface between the layers of the heterostructure is reduced. But at the same time, the magnitude of the miss-mutch induced stresses in the heterostructure, caused by the mismatch of the lattice constants of the materials of the epitaxial layer and the substrate, decreases [18].

Conclusion

In this paper, we analyze the influence of the temperature of growth of epitaxial layers during their growth. We formulate conditions to increase homogeneity of the properties of epitaxial layer. An analytical approach for the analysis of mass and heat transfer is introduced. We introduce an analytical approach for analyzing mass transfer taking into account changes in the process parameters in space and time, as well as taking into account its nonlinearity and changes in the thickness of the epitaxial layer.

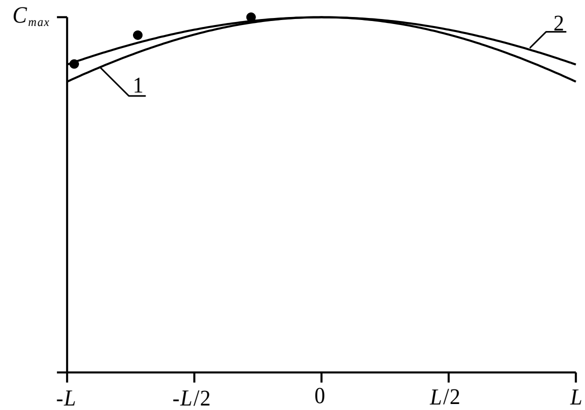

Fig 2: Distributions of concentration of concentration of material of epitaxial layer parallel to interface between layers of heterostructure. Curve 1 corresponds to smaller temperature of growth. Curve 2 corresponds to larger temperature of growth. Points are experimental date from [19].

References

1. Stepanenko IP. Basis of microelectronics. Moscow, Soviet radio, 1980.
2. Gusev VG, M Yu Gusev. Electronics. Moscow, Higher School, 1991.
3. Lachin VI, Savelov NS. Electronics. Rostov-on-Don, Phenics, 2001.
4. Vorob’ev AA, Korabl’ev VV, Yu S Karpov. Semiconductors. 2003; 37(7):98.
5. Sorokin LM, Veselov NV, Shcheglov MP, Kalmykov AE, Sitnikova AA, Feoktistov NA. *et al*. Technical Physics Letters. 2008; 34(22):68.
6. Lundin VV, Sakharov AV, Zavarin EE, Sinitsin MA, Nikolaevв AE, Mikhailovsky GA. *et al*. Tsatsul’nikov. Semiconductors. 2009; 43(7):996.
7. Li Y, Antonuk LE, El-Mohri Y, Zhao Q, Du H, Sawant A, Wang Yi. J Appl. Phys. 2006; 99(6):064501.
8. Chakraborty A, Xing H, Craven MD, Keller S, Mates T, Speck JS. *et al*. J Appl. Phys. 2004; 96(8):4494.
9. Mitsuhara M, Ogasawara M, Sugiura H. J Cryst. Growth, 1998, 183:38.
10. Talalaev RA, Yakovleva EV, Yu S Karpova, Yu N Makarov. J Cryst. Growth, 2001, 230:232.
11. Kozlivsky VV. Modification of semiconductors by proton beams Nauka, Sant-Peterburg, 2003.
12. Z Yu Gotra. Technology of microelectronic devices Radio and communication, Moscow, 1991.
13. Fahey PM, Griffin PB, Plummer JD. Rev. Mod. Phys. 1989; 61(2):289-388.
14. Yu D Sokolov. Applied Mechanics. 1955; 1(1):23-35.
15. Pankratov EL. Applied Nonlinear Dynamics. 2004; 12(3):35-44.
16. Tikhonov AN, Samarskii AA. The mathematical physics equations, Moscow, Nauka, 1972.
17. Carslaw HS, Jaeger JC. Conduction of heat in solids Oxford University Press, 1964.
18. Pankratov EL, Bulaeva EA. Advances in Materials Science and Engineering: An International Journal. 2015; 2(2):1-10.
19. Nazmul AM, Sugahara S, Tanaka M. J Crys. Growth, 2003, 251:303-310.