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DOPED SILICON WITH GALLIUM AND ANTIMUM IMPURITY ATOMS

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Abstract. *In this work, a mathematical model of the concentration distribution of gallium and antimony elements theoretically doped into silicon by diffusion method was studied using the MathCad program. The essence of theoretical calculations and mathematical modeling of the diffusion process is not to waste experiments, to determine in advance the depth of penetration of the impurity atoms into silicon from diffusion, and to plan the experiments and increase the productivity of the results.*

Keywords: *silicon, gallium, antimony, concentration, diffusion, diffusion coefficient.*

INTRODUCTION

The main semiconductor material used in the field of electronics is silicon. Despite the advantages of silicon, such as its large reserves and the availability of standard production technology, the main parameters of silicon, such as the energy of the band gap energy, the mobility of charge carriers, the structure of the energy zone, cannot meet the requirements of the current rapidly developing electronics industry [1-3]. Therefore, today it is of scientific and practical importance to study the effect of binary compounds on the crystal lattice of silicon, which lead to fundamental changes in the properties of silicon [4-5]. The authors [6-7] obtained GaSb layers on various substrates using the modern electron beam epitaxy method and their properties were studied by XRD [8], Raman [9], and TEM [10-11]. The possibility of making high-speed electronic devices [12-14] and the possibility of obtaining infrared detectors [15-16] have been shown. New nanoscale effects [17-19] have been recorded in structures where GaSb layers are limited by one, two or even three sides. However, the modern molecular beam epitaxy method, which is currently used to obtain nanoscale structures, requires both expensive and complex technological processes [20]. In this work, the formation of GaSb binary compound in the Si crystal lattice by diffusion technology was theoretically considered. All calculations were made using MathCad software.

THEORETICAL CALCULATIONS

The authors' works [21-22] shows the diffusion parameters of gallium and antimony elements in silicon.

$$D_i = A \cdot e^{\left(\frac{B[ev]}{kT}\right)} \left[\frac{cm^2}{s}\right] \quad (1)$$

Here, A is a quantity equal to the diffusion coefficient when the temperature is infinite; B-activation energy; D_i-diffusion coefficient.

Table 1.

Elements	A	B
Al	0.317	-3.023
As	8.85	-3.97
B	3.79	-3.645
Bi	1.08	-3.85
Ga	**3.81**	**-3.552**
In	3.13	-3.668
N	200000	-3.24
P	1.03	-3.507
Sb	**40.9**	**-4.158**
Tl	1.37	-3.7

Table 1 and equation (1) can be used to calculate the diffusion coefficient which at the certain temperature.

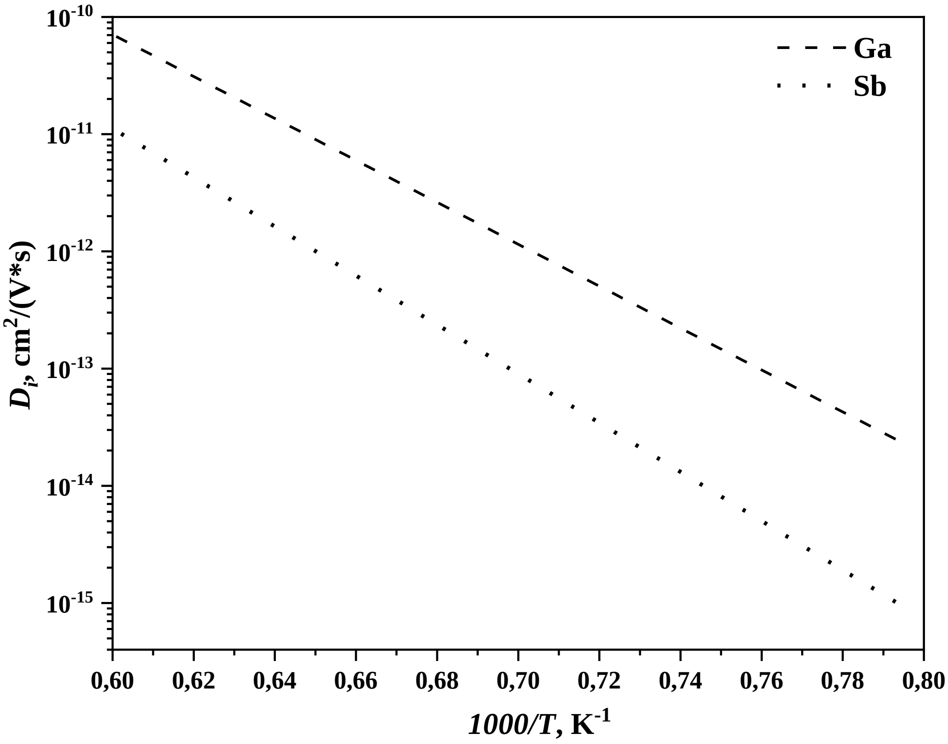


Figure 1. Graph of diffusion coefficients of gallium and antimony elements as a function of temperature.

The graph of the dependence of the concentration of elements on the depth of penetration is determined using the following expression (2):

$$C(x) = C_0 \cdot erfc\left(\frac{x}{2 \cdot \sqrt{D(T) \cdot t}} \right) \qquad (2)$$

Here is $C(x)$—the concentration of the element, C_0—the maximum solubility of the element in silicon, x—is the penetration depth, $D(T)$—the diffusion coefficient, and t—the diffusion time.

The maximum solubility of gallium and antimony elements in silicon at a given temperature can be determined using the following graph:

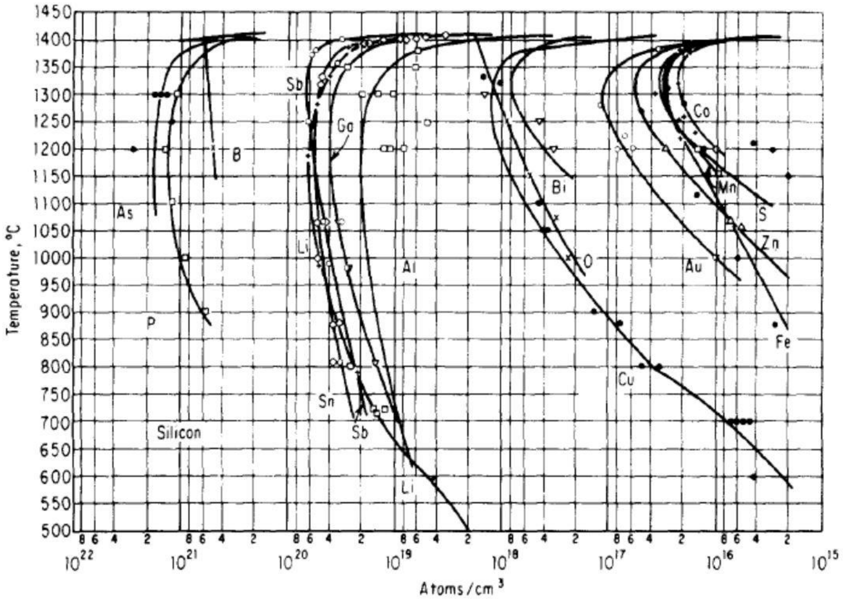


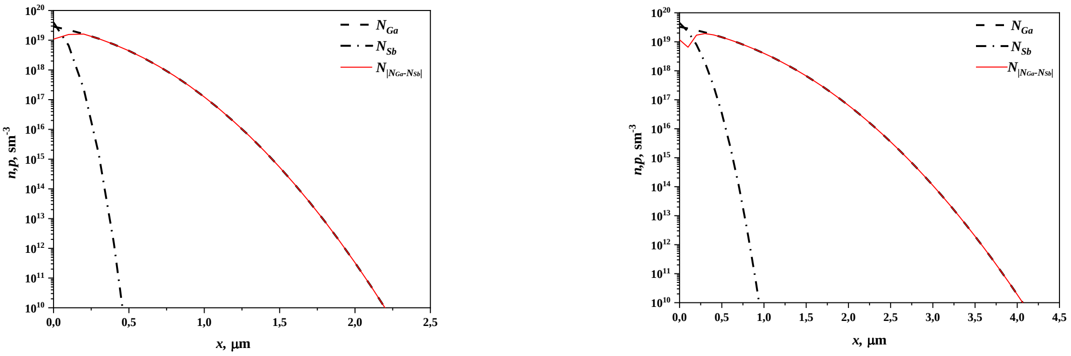
Figure 2. Temperature graph of the solubility of some impurity atoms in silicon.

Using Figure 2, we can construct Table 2 below.

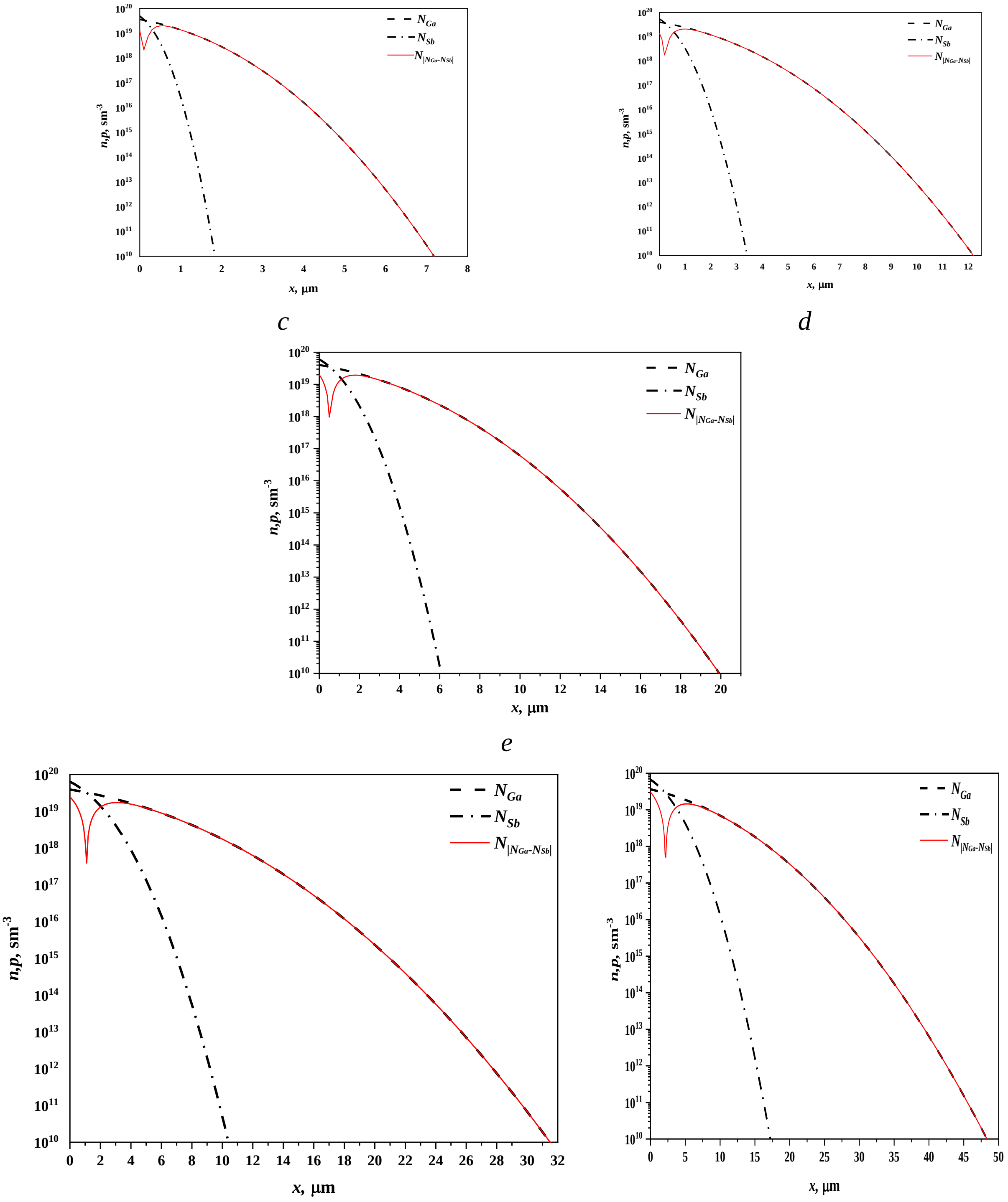
Table 2.

T, °C	$C_0\ (x \cdot 10^{19}),\ cm^{-3}$	
	Sb	Ga
1000	4	3>2
1050	5>4	4>3
1100	5>4	4>3
1150	6>5	4
1200	6>5	4
1250	6	4
1300	7>6	4>3

Using equations (1) and (2) and table 2, we can obtain the distribution of the concentrations of gallium and antimony elements at temperatures of 1000÷1300 °C during the same period of time (5 hours).



a *b*



c

d

e

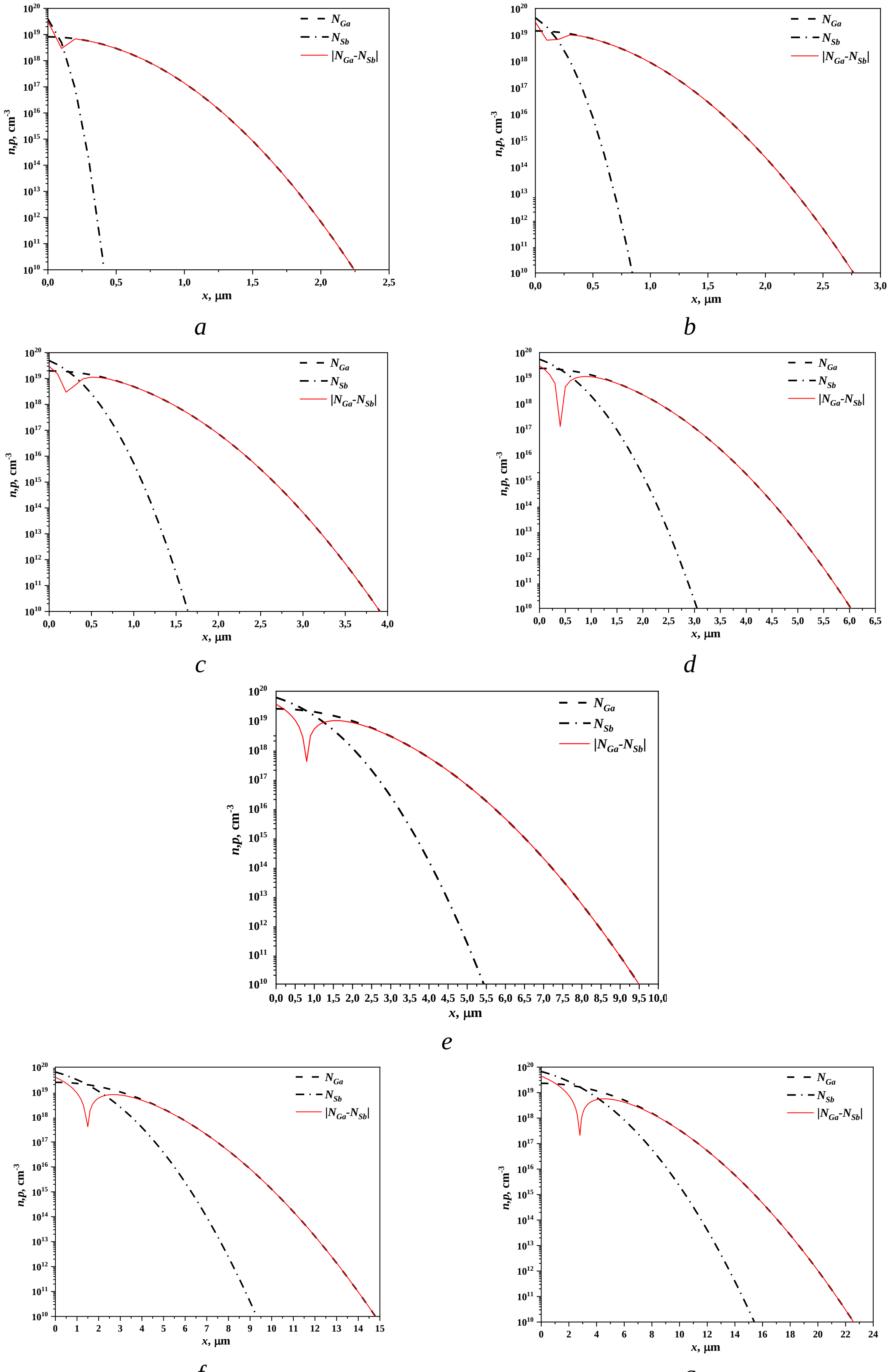
f

g

Figure 3. Depth distribution of concentrations of gallium and antimony atoms entering silicon simultaneously at temperatures of 1000÷1300 °C and during the same time (5 hours).

Figure 3 shows a one-step diffusion, i.e., the situation in which both gallium and antimony atoms are simultaneously diffused into silicon at temperatures of 1000÷1300 °C for 5 hours.

Figure 3 shows the concentration of N_{Ga} - gallium input atoms, N_{Sb} - concentration of antimony input atoms, $N_{|Ga-Sb|}$ - the distribution of the difference in the concentration of gallium and antimony input atoms by depth in silicon. Here, in Fig. 3 *a* – T=1000 °C, *b* – T=1050 °C, *c* – T=1100 °C, *d* – T=1150 °C, *e* – T=1200 °C, *f* – T=1250 ° Theoretically calculated distributions for temperatures C, *g* – T=1300 °C are presented.



a *b*

c *d*

e

f *g*

Figure 4. Depth distribution of gallium and antimony atoms successively introduced into silicon at temperatures of 1000÷1300 °C, during diffusion.

Figure 4 shows two-stage diffusion graphs. In the first stage, gallium atoms were diffused into the silicon sample for 1 hour, and in the second stage, antimony atoms were diffused into the same samples for 4 hours.

Figure 4 shows the concentration of N_{Ga} - gallium input atoms, N_{Sb} - concentration of antimony input atoms, $N_{|Ga\text{-}Sb|}$ - the distribution of the difference in the concentration of gallium and antimony input atoms by depth in silicon. Here, in Fig. 3 *a* – T=1000 °C, *b* – T=1050 °C, *c* – T=1100 °C, *d* – T=1150 °C, *e* – T=1200 °C, *f* – T=1250 °C, *g* – T=1300 °C Theoretically calculated distributions for temperatures are presented.

DISCUSSION

From the graphs in Figures 3 and 4, the depth x where the concentrations of gallium and antimony impurity atoms are equal for both cases is presented in the following table 3.

Table 3

Temperature T, °C	x, µm	
	One-step diffusion	Two-step diffusion
1000	0.07	0.12
1050	0.17	0.19
1100	0.27	0.36
1150	0.57	0.64
1200	1.12	1.22
1250	2.03	2.3
1300	3.65	4.1

It can be seen from Table 3 that at temperatures below 1200 °C, gallium and antimony inclusions can be combined on the silicon surface (x<7 µm). At temperatures of 1200 and 1250 °C, GaSb compounds can be formed in the surface and near-surface areas (x~1.1÷2.3 µm). At a temperature of 1300 °C, the GaSb compound can be formed on the surface, in the subsurface area, and in the volume of silicon (x~3÷5 µm).

CONCLUSION

Based on these calculated results, we can design experiments that we can conduct. The essence of theoretical calculations and mathematical modeling of the diffusion process is that it reduces the number of unnecessary experiments, helps us to achieve the result faster and easier, reduces energy consumption and somewhat reduces costs.

In our future work, we will consider how well the experimental results confirm the theoretical calculations.

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