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REGULAR ARTICLE

Effect of GaSb Compound on Silicon Bandgap Energy

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In this work, the bandgap energy of Si samples doped with impurity atoms of elements Ga (A^{III}) and Sb (B^{V}) by the diffusion method and without impurity atoms was studied. It is known that the bandgap energies of GaSb and Si semiconductors at room temperature are 0.726 and 1.12 eV, respectively. According to the results of the study, it was found that the band gap energies of Ga and Sb-doped and non-doped Si samples are 1.114 and 1.119 eV, respectively. When the samples were further annealed at a temperature of 600 °C, it was observed that the bandgap energy of the samples doped with Ga and Sb decreased to 1.10 eV.

Keywords: Silicon, Gallium, Antimony, Diffusion, Bandgap Energy

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1. INTRODUCTION

The study of the optical properties of semiconductor materials used in the field of electronics, such as group IV elements, binary compounds such as III-V and II-VI, is of both scientific and practical importance [1-3].

III-V compound semiconductors are widely used in the production of high-speed electronic devices due to the high mobility of charge carriers [4-5]. These semiconductors are the main materials for making semiconductor lasers (such as GaAs) and infrared detectors (such as GaSb) due to their proper transition to bandgap energies [6-8]. In addition, III-V compound semiconductors are used in the production of photocells with high efficiency [9].

However, since the production technology of III-V compound semiconductors is complicated and relatively expensive, it is of great practical and scientific interest to obtain them on a semiconductor base with a large supply such as silicon and a well-developed production technology [10-12].

The authors grew a GaSb compound semiconductor layer on the silicon surface using methods such as molecular beam epitaxy [13-14] and solid phase epitaxy [15]. But these modern methods require the use of expensive and complex technological devices compared to the diffusion method.

The authors [16-21] studied their properties by introducing single elements into silicon as impurities atoms, forming their clusters and nanoclusters by diffusion method. However, the properties of the binary compound in silicon by introducing two elements into silicon by diffusion method have not been studied.

The purpose of this work is to study the bandgap energy of the resulting structure by doping the elements Ga and Sb into silicon by diffusion method.

2. RESEARCH

The n-type monocrystalline silicon ($\rho = 1\ \Omega \cdot cm$, $n \sim 5 \cdot 10^{15}\ cm^{-3}$) grown by the Chokhral method was chosen as the used material. Before diffusion process, silicon samples were held in HF acid for 1 ÷ 2 minutes and degreased. The samples were divided into 2 groups. Samples of the first group were diffused Ga and then Sb elements such as impurities atoms into Si at T = 1200 °C for 1 hour and 2 hours, respectively.

Samples of the second group were annealed in two stages (1 hour at temperature T = 1200 °C, repeated for 2 hours at the same temperature) for comparison under identical thermodynamic conditions. The diffusion process was carried out in the AOT-GLS-1750X Vacuum Tube Furnace for Laboratory Material Burning.

3. SPECTROPHOTOMETRIC ANALYSIS

There are various methods for determining the bandgap energy of semiconductors, for example: the dependence of temperature on the relative electrical conductivity of charge carriers, with a decrease in photoconductivity, the optical threshold absorption of the main wavelength, and other methods. However, it is preferable to use the optical absorption method for determining the bandgap energy of semiconductors, because there are no special requirements for the shape and size of the samples, and it is possible to measure with a sufficiently high accuracy.

The essence of the method is that a part of the monochromatic light beam directed to the surface of the semiconductor is reflected from the surface of the sample, a certain part passes through the thickness of the sample, and the rest is absorbed in the thickness of the sample. As a result, the light intensity decreases. The relative change

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in light intensity per unit thickness is called the absorption coefficient. The value of the absorption coefficient depends on the wavelength (λ) of the incident radiation, and $\alpha = f(\lambda)$ function is called the absorption spectrum.

The absorption coefficient α can be calculated using the following equation:

$$\alpha = \frac{1}{d}\ln\frac{(1-R)^2}{T}, \qquad (1)$$

where d is the sample thickness, R is the reflection coefficient, T is the light transmission coefficient.

Equation (1) is valid in case $T < 10\%$. If $T > 10\%$, the relation (2) should be used to calculate the absorption coefficient:

$$T = \frac{(1-R)^2\exp(-\alpha d)}{1-R^2\exp(-2\alpha d)} \qquad (2)$$

To determine the bandgap energy in the optical method, the specific and fundamental absorption of light due to the transition of electrons from the valence band to the conduction band is of the greatest importance. If the energy of the photons (light quanta) is greater than the bandgap energy, there will be a special absorption. Depending on the energy value of the forbidden field, it can appear in the visible or near-infrared region of the spectrum.

When electrons move from the valence band to the conduction band under the influence of light quantum energy, two types of transitions can occur. Transitions involving only photons and electrons are called direct transitions, and transitions involving phonons in addition to photons and electrons are called indirect transitions, i.e., light quantum in absorption, the change in electron energy is accompanied by a change in the energy of the crystal lattice.

The absorption coefficient for semiconductors with the direct transition to the energy zone is written as follows (3):

$$if\ h\nu > E_g,\quad \alpha = B\left(h\nu - \Delta E_g\right)^{1/2} \qquad (3)$$

where ΔE_g is bandgap energy; $h\nu$ is quantum energy of light; B is permanent.

By extrapolating the graph of the $\alpha^2 = f(\lambda)$ function, the intersection of the $h\nu$ axis, it is possible to determine the energy of the area prohibited for semiconductors with the direct transition to the energy zone.

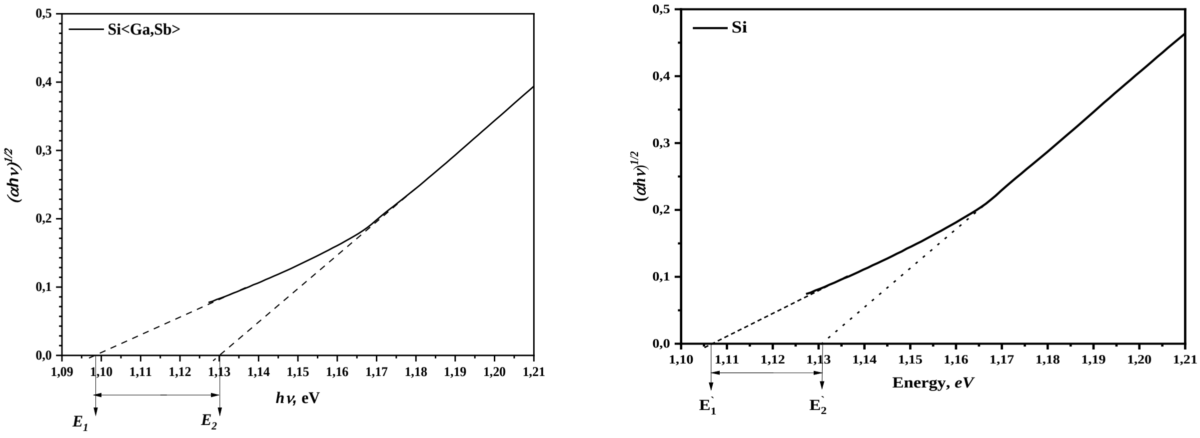
In indirect transition semiconductors in the energy zone, the dependence of the absorption coefficient on photon energy is much more complex, which can be described in general with the following function:

$$if\ \ \Delta E_g - E_{ph} < h\nu < \Delta E_g + E_{ph},\ \alpha^{1/2} = f(h\nu) \qquad (4)$$

where E_{ph} is the energy of the phonograph in semiconductors with indirect transition to the energy zone [22].

It is known that the bandgap energies at room temperature of the GaSb and Si semiconductors are 0.726 (direct transition) and 1.12 eV (indirect transition) respectively.

Expression was used (4) equation because the used material was silicon (Fig. 1).



a) b)

Fig. 1 – Spectrophotometer analysis of samples: a) Group I sample (Si<Ga,Sb>); b) Group II sample(Si).

Group I and group II samples are presented with results obtained in a spectrophotometer after diffusion. In the Fig. 1(a) – $E_1 = E_{g,Si<Ga,Sb>} - E_{ph}$ and $E_2 = E_{g,Si<Ga,Sb>} + E_{ph}$ are equal to 1.098 and 1.13 relatively. In the Fig. 1(b) – $E_1^{`} = E_{g,Si}^{`} - E_{ph}^{`}$ and $E_2^{`} = E_{g,Si} + E_{ph}^{`}$. These results and values were found to be 1,114 and 1,119 eV respectively. The reason why the forbidden energy gap of the Group I sample after diffusion did not differ greatly from the forbidden energy gap of pure silicon is because GaSb binary compounds were formed at a low concentration.

Group I samples were additionally annealed at temperatures T = 600, 700, 800, 900, 1000 °C. Due to the fact that the boiling point of GaSb compound semiconductor was T ~ 713 °C and the diffusion coefficient of Ga entrance into Si was greater than that of Sb entrance, the additional annealing of group I samples at T = 700 °C and higher showed practically the same value (~ 1,12 eV) as the band gap width of pure silicon sample. It turned out to be equal to $E_{g,Si<Ga,Sb>}^{600} = 1.10$ eV at additional annealing of group I samples at T = 600 °C (Fig. 2).

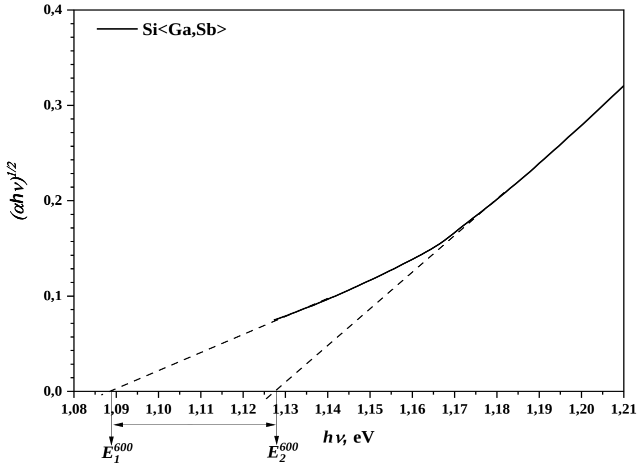


Fig. 2 – Spectrophotometric result obtained after additional annealing of group I sample at $T = 600$ °C

To design a new material model in the form of $Si_{1-x}(GaSb)_x$, an 8-atom supercell with a 6-angle geometry is used [23-25]. The band gap energy of a new material being developed is calculated according to Vegard's law as follows:

$$E_{g,Si_{(1-x)}GaSb_x} = (1-x)\cdot E_{g,Si} + x\cdot E_{g,GaSb} \tag{5}$$

where, x is the molar fraction of the substance, the bandgap energy of silicon single crystal at room temperature is equal to $E_{g,Si} = 1{,}12\ eV$, bandgap energy of antimonide gallium single crystal at room temperature is equal to $E_{g,GaSb} = 0{,}726\ eV$. If 0, 0.5, 1 takes the values of x (5) it can be seen from the expression that the appropriate relation takes the values

$$E_{g,Si_{(1-x)}GaSb_x} = (1-0)\cdot E_{g,Si} + 0 = 1{,}12\ eV\ ,$$

$$E_{g,Si_{(1-x)}GaSb_x} = E_{g,Si_{0,5}GaSb_{0,5}} = (1-0{,}5)\cdot 1{,}12 + 0{,}5\cdot 0{,}726 = 0{,}923\ eV\ ,$$

$$E_{g,Si_{(1-x)}GaSb_x} = (1-1)\cdot E_{g,Si} + 1\cdot E_{g,GaSb} = 0{,}726\ eV$$

If we change it at $x = 0 \to 1$ a rate of 0.05, we get the following Table 1.

Table 1 – Table of quantitative variation of bandgap energy of $Si_{1-x}(GaSb)_x$ alloy

x	0	0.05	0.1	0.15	0.2	0.25	0.3	0.35	0.4	0.45	0.5
$E_{g,Si_{(1-x)}GaSb_x}$ [eV]	1.12	1.1003	1.0806	1.0609	1.0412	1.0215	1.0018	0.9821	0.9624	0.9427	0.923
x	0.55	0.6	0.65	0.7	0.75	0.8	0.85	0.9	0.95	1.0	
$E_{g,Si_{(1-x)}GaSb_x}$ [eV]	0.9033	0.8836	0.8639	0.8442	0.8245	0.8048	0.7851	0.7654	0.7457	0.726	

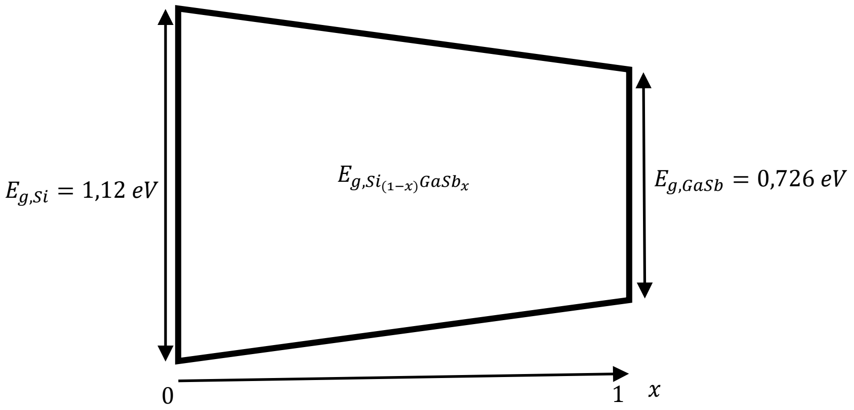


Fig. 3 – According to Vegard's law, the quantitative change in bandgap energy of the alloy

The bandgap energy of the group I sample is equal when additionally heated at $T = 600$ °C. Using Vegard's law, the quantitative fraction of Si and the formed GaSb binary compound was calculated. And according to it was determined.

4. SUMMARY

When samples of group I were additionally heated at temperatures T = 700, 800, 900, 1000 °C, due to the difference in the diffusion coefficients of Ga and Sb inputs (at a certain temperature), GaSb binary compound was not formed in the Si sample. At the temperature T = 600 °C, it was found that the GaSb binary compound was formed in Si in a small amount, as an example, it can be shown that the bandgap energy of the group I sample decreased to 1.10 eV. The formation of Si type alloy on the surface and near the surface can be done using Vegard's law. It can be seen that the GaSb binary compound is formed in the surface and near-surface area of Si, and the bandgap energy of Si can be controlled by using this GaSb-like $A^{III}B^{V}$ binary compound layers.

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Вплив сполуки GaSb на ширину забороненої зони кремнію

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Досліджена ширина забороненої зони зразків Si, легованих домішковими атомами елементів Ga (AIII) і Sb (BV) дифузійним методом і без домішкових атомів. Відомо, що ширина забороненої зони напівпровідників GaSb і Si при кімнатній температурі становить 0,726 і 1,12 еВ відповідно. Установлено, що щирина забороненої зони зразків Ga та Sb легованого та нелегованого Si становить 1,114 та 1,119 еВ відповідно. Під час подальшого відпалу матеріалів при температурі 600 °C було виявлено, що ширина забороненої зони легованих Ga та Sb зразків зменшується до 1,10 еВ.

Ключові слова: Кремній, Галій, Антимонід, Дифузія, Ширина забороненої зони.