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Change in the Concentration of Oxygen Atoms in Silicon During the Diffusion of Antimony and Gallium Atoms

Bobir Isakov[a)], Xalmurat Iliev, Bakhrom Abdurkhamanov, Giyosiddin Kushiev, Zabarjad Umarxodjayeva, Islambek Kazakbaev

Tashkent state technical university named after Islam Karimov, Tashkent, Uzbekistan

[a)] *Corresponding author: bobir6422isakov@gmail.com*

Abstract. In this work, the influence of impurity atoms of gallium and antimony on the concentration of optically active oxygen in the silicon lattice is investigated. It is shown that the oxygen concentration in silicon samples doped with gallium decreases by 87.2%, doped with antimony decreases by 90.5%, and in the case of doping with gallium and antimony simultaneously only by 28.7%. These results can be explained by the chemical interaction of gallium and antimony atoms, which leads to the restoration of the oxygen concentration in optical active centers.

INTRODUCTION

The diffusion of impurity atoms into silicon is one of the key processes determining the formation of the required electrical and structural properties of materials used in modern microelectronics [1–6]. Controlled introduction of alloying elements allows for targeted modification of charge carrier concentration, potential distribution, and conductivity parameters, which forms the basis for the creation of highly efficient semiconductor devices.

In recent decades, particular attention has been paid to the study of nanoclusters of impurity atoms formed in silicon during diffusion. Analysis of their structure, energy state, and evolution under various thermal conditions has shown that such nanoclusters have a significant impact on recombination processes, carrier mobility, and the stability of electrical characteristics [7–12]. These studies have led to the discovery of a number of new physical phenomena related to the self-organization of impurity complexes, their interaction with crystal lattice defects, and their influence on charge transport mechanisms. These results open up prospects for the creation of new generations of semiconductor structures with improved performance parameters.

EXPERIMENTAL RESEARCH

The behavior of Ga and Sb atoms during sequential diffusion into silicon and the possibility of forming binary compounds within the silicon lattice are of great scientific and practical interest. This paper demonstrates the formation of Ga and Sb binary compounds in the silicon lattice based on a study of its optical properties.

Samples of industrial silicon grade KEF-1 were selected as the starting material, from which samples measuring 6×2×1 mm^3 were manufactured. The surface of the initial samples was polished using diamond paste and cleaned with an ammonium peroxide solution before diffusion. The diffusion process was carried out in a single-zone vacuum tube furnace of the type MG17-60/300 in two stages. In the first stage, the diffusion of gallium (Ga) impurity into silicon was carried out at a temperature of T=1100 °C for 60 minutes. In the second stage, the diffusion of antimony (Sb) impurity was carried out at a temperature of T=1250 °C for 180 minutes. At each stage of diffusion, control silicon samples (without impurity) were annealed under the same conditions. After diffusion, the samples were mechanically polished using diamond paste grade W-0.25.

According to the processing conditions, the samples were divided into three groups (Figure 1).

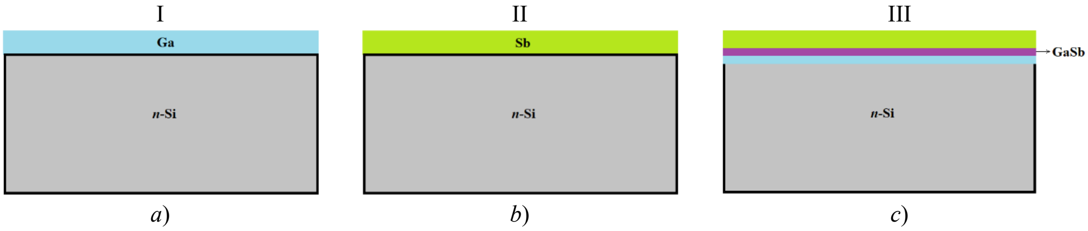

FIGURE 1. Structure of silicon samples diffusion-doped with atoms of gallium (*a* – group I), antimony (*b* – group II) and sequentially gallium and antimony (*c* – group III).

Group *I*. (Fig. 1. A). In the first stage, samples of the initial KEF-1 material were doped with gallium atoms at T=1100 °C; t=3 h. In the second stage, these samples were subjected to repeated heat treatment at T=1250 °C; t=1 h.

Group *II*. (Fig. 1. B). In the first stage, the initial material KEF-1 was subjected to heat treatment at T=1100 °C; t=3 h. In the second stage, these samples were doped with antimony atoms at T=1250 °C; t=1 h.

Group *III*. (Fig. 1. C). In the first stage, samples of the initial KEF-1 material were doped with gallium atoms at T=1100 °C; t=3 h. In the second stage, these samples were additionally doped with antimony atoms at T=1250 °C; t=1 h.

RESULTS AND DISCUSSION

In silicon samples, the concentration of optically active oxygen (N_O^{OPT}) was determined by the well-known formula [13-16], using IR absorption spectra in the region of λ=9041 nm

$$N_O^{OPT} = 3,3\cdot 10^{17}\cdot\frac{1}{d}\cdot\ln\frac{I}{I_0} \tag{1}$$

where: I and I_0 are the intensities of incident and transmitted light, d is the thickness of the silicon sample.

Figure 2 (curve 1) shows the absorption spectrum of the original silicon sample. In the spectral region λ=9041 nm there is an absorption peak associated with optically active oxygen [17-20].

Change in the content of optically active oxygen after diffusion of gallium atoms into silicon.

For control samples – Si<control>, using the data in Fig. 2, curve 1, the oxygen concentration was:

$$N_O^{OPT(control)} = 3,3\cdot 10^{17}\cdot\frac{1}{d}\cdot\ln\frac{I}{I_0} = 8\cdot 10^{17}\ cm^{-3} \tag{2}$$

For samples of group I – Si<Ga>, using the data in Fig. 2, curve 2, the oxygen concentration was:

$$N_O^{OPT(Ga)} = 3,3\cdot 10^{17}\cdot\frac{1}{d}\cdot\ln\frac{I}{I_0} = 10^{17}\ cm^{-3} \tag{3}$$

Reduction of oxygen concentration in Si<Ga> samples relative to the control:

$$\frac{N_O^{OPT(control)} - N_O^{OPT(Ga)}}{N_O^{OPT(control)}}\cdot 100\% = \frac{8\cdot 10^{17} - 1,025\cdot 10^{17}}{8\cdot 10^{17}}\cdot 100\% = 87,2\% \tag{4}$$

Thus, doping silicon samples with gallium atoms results in an 87.2% reduction in oxygen concentration. These results can be explained by the chemical interaction of gallium and oxygen atoms, which leads to a decrease in the absorption peak magnitude.

Change in the content of optically active oxygen after diffusion of antimony atoms into silicon.

For samples of group II - Si<Sb>, using the data in Fig. 2, curve 3, the oxygen concentration was:

$$N_O^{OPT(Sb)} = 3,3\cdot 10^{17}\cdot\frac{1}{d}\cdot\ln\frac{I}{I_0} = 7,6\cdot 10^{16}\ cm^{-3} \tag{5}$$

Reduction in oxygen concentration in samples of group II - Si<Sb> relative to the control:

$$\frac{N_O^{OPT(control)} - N_O^{OPT(Sb)}}{N_O^{OPT(control)}}\cdot 100\% = \frac{8\cdot 10^{17} - 7,6\cdot 10^{16}}{8\cdot 10^{17}}\cdot 100\% = 90,5\% \tag{6}$$

Thus, doping silicon [21-23] with antimony impurity atoms leads to a 90.5% decrease in oxygen concentration. These results can also be explained by the chemical interaction of antimony and oxygen atoms in optically active centers; however, due to the high solubility of antimony impurity atoms in silicon at the diffusion temperature, the interaction effect is more pronounced.

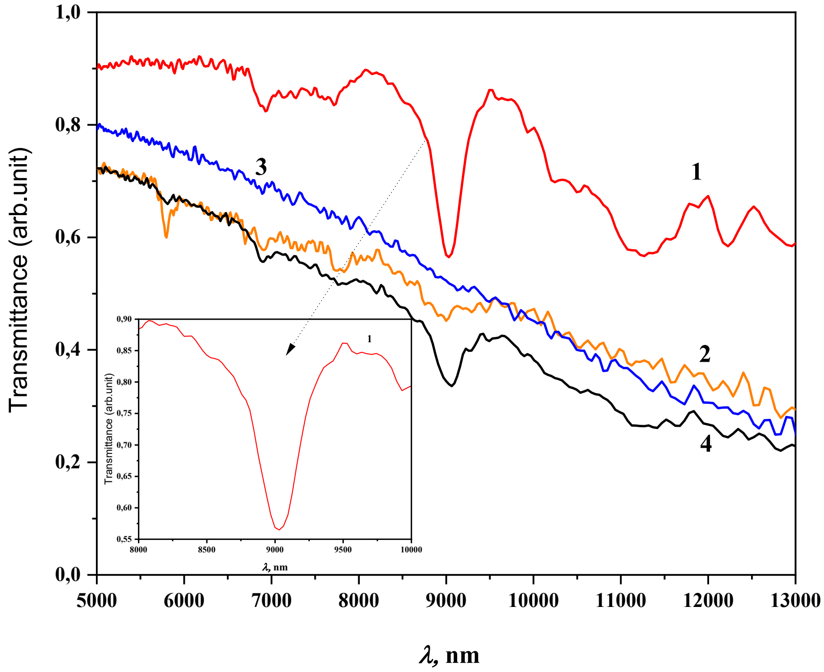

FIGURE 2. Spectral dependences of light transmission in samples: 1 - initial silicon KEF-1; 2 - Si<Ga>; 3 - Si<Sb>; 4 - Si<Ga,Sb>.

Change in optically active oxygen content after diffusion of gallium and antimony atoms into silicon.

For samples of group III - Si<Ga, Sb> (doped first with gallium and then with antimony), using the data in Fig. 2, curve 4, the oxygen concentration was:

$$N_O^{OPT(GaSb)} = 3{,}3 \cdot 10^{17} \cdot \frac{1}{d} \cdot \ln \frac{I}{I_0} = 5{,}7 \cdot 10^{17}\ cm^{-3} \tag{7}$$

Reduction in oxygen concentration in samples of group III - Si<Ga, Sb> relative to the control:

$$\frac{N_O^{OPT(control)} - N_O^{OPT(GaSb)}}{N_O^{OPT(control)}} \cdot 100\% = \frac{8 \cdot 10^{17} - 5{,}706 \cdot 10^{17}}{8 \cdot 10^{17}} \cdot 100\% = 28{,}7\% \tag{8}$$

Thus, doping silicon with antimony and gallium atoms leads to a 28.7% decrease in oxygen concentration.

The study results show that the change in optically active oxygen concentration after diffusion of gallium and antimony impurity atoms is significantly smaller than after doping with gallium or antimony alone. Furthermore, the change in oxygen concentration during diffusion processes over a period of only 4 hours due to the formation of thermal donors can be ignored [10].

This effect can be explained by the fact that gallium and antimony atoms neutralize each other's action due to the formation of binary quasi-molecular compounds such as Si_2GaSb in the silicon lattice.

CONCLUSIONS

The studies showed that the oxygen concentration in silicon samples depends significantly on the type of dopant. Specifically, in gallium-doped silicon, the oxygen content decreases by 87.2%, while with antimony doping, the decrease reaches 90.5%. However, with the combined introduction of gallium and antimony, the oxygen concentration decreases by only 28.7%, indicating a fundamentally different nature of the physicochemical processes occurring.

The obtained results can be interpreted through the mechanism of chemical interaction between gallium and antimony atoms, which facilitates the partial restoration of oxygen concentration in optically active centers. It is assumed that the formation of binary nanoclusters of the Si_2GaSb type in the silicon lattice leads to a change in the local chemical environment and a redistribution of oxygen-containing complexes. To confirm this hypothesis, in-depth studies of the electrophysical, optical, and photoelectric characteristics of materials containing binary compounds are necessary.

The presence of Si_2GaSb clusters in the silicon crystal structure can significantly affect charge carrier mobility, recombination characteristics, band gap width, and thermal stability. Such structural modifications open up new prospects for the use of doped silicon in a number of high-tech applications. In particular, materials with binary Si_2GaSb impurity complexes are of interest for infrared photonics, sensors, terahertz electronics, and the development of energy-saving power and high-voltage semiconductor devices requiring high stability and controlled conductivity.

Thus, the Si_2GaSb nanostructures formed in silicon as a result of diffusion processes can be considered as a promising platform for the creation of new functional materials with improved optical and electrophysical properties.

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