Influence of Impurity Atoms of Gallium and Antimony on the Concentration of Optically Active Oxygen in the Silicon Lattice

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Annotation: The effect of impurity atoms of gallium and antimony on the concentration of optically active oxygen in the silicon lattice is studied. It is shown that the oxygen concentration in silicon samples doped with gallium decreases by 87.2%, doped with antimony decreases by 99.2%, and in the case of doping with gallium and antimony decreases 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.

Keywords: diffusion, silicon, gallium, antimony, oxygen.

The diffusion of impurity atoms into silicon plays an important role in obtaining materials with the required properties in microelectronics [1–4]. To date, the study of nanoclusters of impurity atoms in silicon obtained by the diffusion method led to the discovery of a number of physical phenomena [5-7].

The behavior of Ga and Sb atoms during their successive diffusion into silicon and the possibility of the formation of binary compounds inside the silicon lattice is of great scientific and practical interest. In this work, the formation of a binary compound of Ga and Sb in a silicon lattice was shown based on the study of its optical properties.

Samples of industrial silicon grade KEF-1 were chosen as the initial material, from which samples 6 × 2 × 1 mm³ in size were made. The surface of the initial samples was polished using diamond paste and cleaned in peroxide-ammonia solution before diffusion. The diffusion process was carried out in a single-zone vacuum tube furnace brand MG17-60/300 in two stages. At the first stage, gallium (Ga) impurities were diffused into silicon at a temperature T=1100°C for 60 minutes. At the second stage, the diffusion of the antimony (Sb) impurity was carried out at a temperature T=1250 °C for 180 minutes. At each stage of diffusion under the same conditions, control samples of silicon (without impurities) were annealed. After diffusion, the samples were subjected to mechanical polishing using W-0.25 diamond paste.

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

Group I. (Fig 1.a). At the first stage, samples of the initial material KEF-1 were doped with gallium atoms at T=1100°C within t=3 hours. At the second stage, these samples were subjected to repeated heat treatment at T=1250°C within t=1 hour.

Group II. (Fig.1.b). At the first stage, the initial material KEF-1 was subjected to heat treatment at T=1100 °C within t=3 hours. At the second stage, these samples were doped with antimony atoms at T=1250°C within t=1 hour.

Group III. (Fig.1.c). At the first stage, samples of the KEF-1 initial material were doped with gallium atoms at T=1100°C within t=3 hours. At the second stage, these samples were additionally doped with antimony atoms at T=1250°C within t=1 hour.

In silicon samples, the concentration of optically active oxygen (N_{O_{opt}}) was determined by the well-known formula [8-10], using the IR absorption spectra in the region λ=1106 sm⁻¹.
\[ N_o^{\text{OPT}} = 3.03 \cdot 10^{17} \cdot \frac{1}{d} \cdot \ln \frac{I}{I_0} \]

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

Fig. 2 (curve 1) shows the absorption spectrum of the initial silicon sample. In the spectral region \( \lambda = 1106 \text{ sm}^{-1} \), there is an absorption peak associated with optically active oxygen [11-13].

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

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

\[ N_o^{\text{OPT}} = 3.03 \cdot 10^{17} \cdot \frac{1}{d} \cdot \ln \frac{I}{I_0} = 8 \cdot 10^{17} \text{ cm}^{-3} \]

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

\[ N_o^{\text{OPT}} = 3.03 \cdot 10^{17} \cdot \frac{1}{d} \cdot \ln \frac{I}{I_0} = 10^{17} \text{ cm}^{-3} \]

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

\[ \frac{N_o^{\text{OPT(KONT)}} - N_o^{\text{OPT(Ga)}}}{N_o^{\text{OPT(KONT)}}} \cdot 100\% = \frac{8 \cdot 10^{17} - 1.025 \cdot 10^{17}}{8 \cdot 10^{17}} \cdot 100\% = 87.2\% \]

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

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

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

\[ N_o^{\text{OPT}} = 3.03 \cdot 10^{17} \cdot \frac{1}{d} \cdot \ln \frac{I}{I_0} = 6.343 \cdot 10^{15} \text{ cm}^{-3} \]

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

\[ \frac{N_o^{\text{OPT(KONT)}} - N_o^{\text{OPT(Sb)}}}{N_o^{\text{OPT(KONT)}}} \cdot 100\% = \frac{8 \cdot 10^{17} - 6.343 \cdot 10^{15}}{8 \cdot 10^{17}} \cdot 100\% = 99.2\% \]

Thus, silicon doping with antimony impurity atoms leads to a decrease in the oxygen concentration by 99.2%. These results can also be explained by the chemical interaction of antimony and oxygen atoms in optical active centers; however, due to the high solubility of impurity antimony atoms in silicon at the diffusion temperature, the interaction effect is more pronounced.

3. Change in the content of optically active oxygen 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 of Fig. 2, curve 4, the oxygen concentration was:

\[ N_o^{\text{OPT}} = 3.03 \cdot 10^{17} \cdot \frac{1}{d} \cdot \ln \frac{I}{I_0} = 5.7 \cdot 10^{17} \text{ cm}^{-3} \]
Decrease in oxygen concentration in samples of group III - Si<Ga, Sb> relative to the control:

\[
\frac{N_{O}^{\text{OPT (Контр)}} - N_{O}^{\text{OPT (GaSb)}}}{N_{O}^{\text{OPT (Контр)}}} \cdot 100\% = \frac{8 \cdot 10^{17} - 5.706 \cdot 10^{17}}{8 \cdot 10^{17}} \cdot 100\% = 28.7\%
\]

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

It can be seen from the results of the study that the change in the concentration of optically active oxygen after the diffusion of impurity atoms of gallium and antimony is much less than when doped with only gallium or antimony. In this case, one can neglect the change in the oxy-gen concentration during diffusion processes for only 4 hours due to the appearance of thermal donors [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 quasimolecular compounds of the Si₂GaSb type in the silicon lattice.

It is shown that the oxygen concentration in silicon samples doped with gallium decreases by 87.2%, doped with antimony decreases by 99.2%, 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. To confirm this assumption, it is necessary to carry out more detailed studies of the electrical and photoelectric properties of the obtained materials with binary compounds of impurity atoms. The presence of binary compounds in the silicon lattice should lead to a change in the electrical properties of the material, for example, to a change in the mobility of carriers and the band gap.

**Conflict of interest**

The authors declare that they have no conflict of interest.

**Literature**

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Fig. 1. The structure of silicon samples diffusion-doped with gallium atoms:
(a - group I), antimony (b - group II) and sequentially with gallium and antimony (c - group III).

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