

## THE INTERACTION BETWEEN IMPURITIES T-ION WITH THE ASSOCIATED STATES OF OXYGEN IN SILICON

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### ABSTRACT

In this paper, the interaction of impurities of transition elements with associated states of a technological impurity (oxygen) in silicon, was studied by infrared spectroscopy. It was found that the diffusion of chromium, manganese or cobalt atoms into silicon leads to a decrease in the concentration of optically active free (interstitial) oxygen by 10-30%. It is shown that high-temperature processing of silicon samples at

1100°C leads to the precipitation of oxygen atoms and the formation of particles of the SiO<sub>2</sub> or SiO<sub>4</sub> type, as a result of which the N<sub>o</sub><sup>opt</sup> decreases by 45-50%. Doping of the samples, previously subjected to heat treatment, with T-ion atoms leads to a further decrease in N<sub>o</sub><sup>opt</sup> by 8-10%.

**KEYWORDS:** spectroscopy, silicon, defect, associated states doping of the impurity, oxygen, chromium, manganese, cobalt,

### INTRODUCTION

In recent years for the controlled formation of defect structure in silicon using the impurity transition elements (T -ions), creating a forbidden zone of silicon a number of deep levels. Earlier it was found that these specially introduced impurities interact with various uncontrolled impurities in the process of technological treatments.<sup>[1-6]</sup> In addition, it was found that various high -temperature treatments (HTT) lead to a change in the defect structure of single -crystal silicon.<sup>[3]</sup> This leads to the formation of various associated states

of technological impurities, for example, oxygen or carbon atoms in silicon. Depending on the treatment temperature, new phase state of technological impurities - particles such as  $\text{SiO}_2$  or  $\text{SiO}_4$  - are formed.<sup>[3]</sup>

In connection with this, we studied the interaction between impurities T-ions, in particular, chromium, manganese or cobalt, with bound (associated) states of oxygen atoms in silicon by means of infra-red (IR) spectroscopy.

## MATERIALS AND METHODS

The initial samples were n-type and p-type silicon grown by the Czochralski method with a concentration of optically active oxygen  $N_o^{\text{opt}} = 6 \cdot 10^{17} \div 1.2 \cdot 10^{18} \text{ cm}^{-3}$  and carbon  $N_c^{\text{opt}} = 2 \cdot 10^{16} \text{ cm}^{-3}$ , the thickness of the polished samples was 1÷2 mm. The contents of oxygen  $N_o^{\text{opt}}$  and carbon  $N_c^{\text{opt}}$  was estimated from the infrared absorption spectra at the 1100  $\text{cm}^{-1}$  region (oxygen band) and 610  $\text{cm}^{-1}$  (carbon band) measured on the infrared spectrophotometer Specord –IR75 in a two-beam scheme at 300 K using the formulas<sup>[4]</sup>:

$$N_o^{\text{opt}} = 3.3 \cdot 10^{17} \cdot 1/d \cdot \ln I / I_0$$

$$N_c^{\text{opt}} = 1.1 \cdot 10^{17} \cdot 1/d \cdot \ln I / I_0$$

where  $I$  and  $I_0$  are the intensities of the incident and transmitted light,  $d$  is the thickness of the samples under study.

As a reference sample, used was a polished oxygen-free Si of the same thickness as that of the sample with  $N_o^{\text{opt}} \leq 10^{16} \text{ cm}^{-3}$ ,  $N_c^{\text{opt}} = 5 \cdot 10^{15} \text{ cm}^{-3}$ .

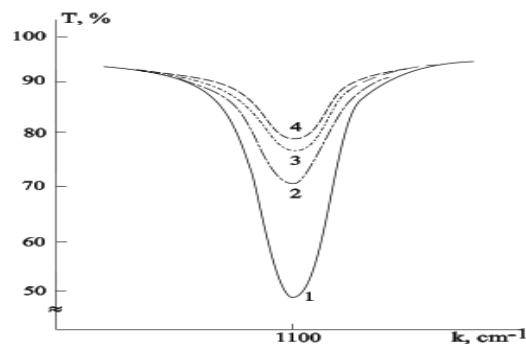
## RESULTS AND DISCUSSION

To study the interaction of T-ion impurities with the associated states of oxygen atoms, we fabricated samples subjected to high -temperature treatment at a temperature of 1100°C for 12 hours.

Further, after measuring  $N_o^{\text{opt}}$  and  $N_c^{\text{opt}}$  in the initial and heat treated samples, impurities of chromium, manganese or cobalt, were introduced in them by the diffusion method from a layer of a corresponding metal sputtered in a vacuum in the temperature range 900-1250 ° C for 20 hours.

Then again,  $N_o^{opt}$  and  $N_c^{opt}$  were measured the results of these measurements are shown in Fig. 1, where typical infrared absorption spectra of one of the impurities of transition ions - chromium are given.

From the analysis of the obtained results it follows that after the introduction of a chromium impurity into silicon of both n -type and p-type, a decrease in the value of  $N_o^{opt}$  is observed in comparison with the control samples heat -treated under the same conditions as the diffusion of chromium (Fig. 1, curves 1 –4). It should be noted that the decrease of  $N_o^{opt}$  depends on the concentration of electrically active chromium atoms and is 10–30% (curves 1 and 2), and the  $N_c^{opt}$  value remains almost unchanged.



**Fig. 1: Typical spectra of the infrared absorption of silicon doped with Cr.**

1. The initial (control) silicon,
2. n-Si<Cr>,
3. n-Si + heat treatment,
4. n-Si<Cr> with preliminary heat treatment

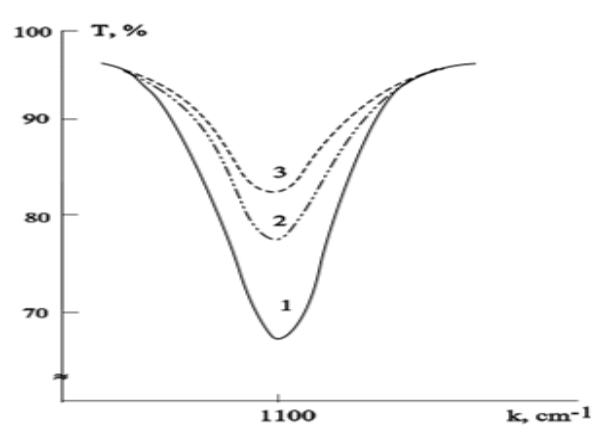
In slowly cooled samples of silicon doped with chromium, the effect of changing  $N_o^{opt}$  was not detected. Analogous infrared absorption spectra were also observed for manganese and iron impurities with a small difference.

From the surface of silicon samples previously subjected to high -temperature treatment (HTT), then doped with one of the T-ions, the mechanically broken layers were removed by grinding. Further, in these samples were measured resistivity spectra and the IR absorption. For comparison, control samples were subjected to repeated heat treatment under the same conditions as diffusion of T -ions ( $T=900\div 1250^{\circ}\text{C}$  for 20 hours), as well as samples doped with T ions without preliminary heat treatment. The results of these studies showed that the

introduction of impurities of transition ions in the n -type silicon leads to an insignificant change in the value of the resistivity, regardless of the initial sample completed the preliminary high-temperature treatment or not. In samples of p-type silicon, a significant increase in the resistivity is observed and in these samples with impurities of transition ions, subjected to preliminary heat treatment, the increase  $\rho$  several times less than in samples that have not undergone preliminary heat treatment.

Earlier<sup>[2]</sup> it was shown that under high temperature treatment at  $T=1100\text{ }^{\circ}\text{C}$  occurs the precipitation of oxygen atoms, i.e. free interstitial oxygen passes into the second phase with the formation of  $\text{SiO}_2$  particles. Impurity of transition ions when introduced into the pre-heat-treated silicon, apparently, is deposited on the  $\text{SiO}_2$  clusters, with the result that they, perhaps, lose their electrical activity. This explains the difference in the magnitude change of resistivity in the samples p-Si with impurities of transition ions with a preliminary high temperature treatment and without it.

Measurements of the IR absorption spectra in heat -treated silicon samples showed that high-temperature treatment at  $1100^{\circ}\text{C}$ , accompanied by the precipitation of oxygen atoms, leads to a significant decrease in  $N_{\text{o}}^{\text{opt}}$  by an optic of 45-50% (Fig.1, curve3). It was shown above that the introduction of impurities of T -ions in Si leads to a decrease in the concentration of optically active oxygen  $N_{\text{o}}^{\text{opt}}$ . The doped of silicon samples preliminarily subjected to heat treatment by chromium atoms leads to a further decrease in  $N_{\text{o}}^{\text{opt}}$  by 8-10%, which is explained by the interaction of



**Fig. 2: Typical spectra of the infrared absorption of silicon doped with Co.**

- 1 - The initial (control) silicon,
- 2- n-Si<Co>,

3- n-Si after heat treatment,

Chromium atoms with oxygen precipitates. (Fig.1, curve 4).

A similar effect was not observed in samples previously subjected to high - temperature treatment, and then doped with an admixture of cobalt (Fig. 2, curves 1 -or manganese. This is probably due to the peculiarities of the interaction of various impurities of T-ions with bound states of oxygen atoms.

## CONCLUSIONS

Thus, it has been shown that doping of silicon with impurities of T ions leads to a decrease in the concentration of optically active oxygen  $N_o^{opt}$  by 10-30%, depending on the impurity introduced and its concentration.

It was also found that the preliminary heat treatment of silicon samples at 1100°C for 12 hours leads to the precipitation of oxygen with the formation of  $SiO_2$  particles. In this case  $N_o^{opt}$  is decreases by 45-50%.

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