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**REGULAR ARTICLE**

# Nickel Clusters in the Silicon Lattice

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The paper studies the gettering properties of nickel clusters in the silicon lattice. The gettering properties of nickel clusters were studied in various states, i.e., in original (reference) samples, as well as in samples with additionally doped interstitial and lattice site impurity atoms of sulfur and manganese. The electrophysical and photoelectric parameters were studied using modern instrumentation: INFRAM-I-type infrared microscope, IKS-21 and scanning electron microscope SEM (Oxford Instruments ZEISS EVOMA10), IKS-21. A new technology has also been proposed that makes it possible to getter harmful impurities; it is recommended for widespread use in the electronics industry and scientific research institutes for the production of materials with stable parameters and the development of fundamentally new devices.

**Keywords**: Silicon, Nickel, Cluster, Thermal donors, Temperature, Gettering, Diffusion, lifetime.

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## 1. INTRODUCTION

Gettering properties of clusters of impurity atoms of nickel were discussed in [1-3]. Impurity atoms of nickel have a high diffusion coefficient ($D = 10^{-5}$ cm²/second) and are characterized by high solubility ($N = 10^{18}$ cm$^{-3}$) at T = 1200°C. Besides that, they could be interesting due to their power to form clusters characterized by their ability to remove defects [4, 5]. Earlier [6] it was demonstrated that the share of electroactive atoms of nickel in silicon could be $N = 5 \times 10^{14}$ cm$^{-3}$. The majority of dopant atoms of nickel (99.999%) are believed to be in electrically neutral state.

There are several techniques for removing impurities [7-10] from material, for example, the ion implantation, laser processing, etc., but it should be noted that the above methods are expensive, require the presence of some sophisticated technological equipment. Moreover, electrical parameters change significantly in times of processing of material. Therefore, developing an alternative impurity removal method that would not significantly affect the electrical parameters of the processed material becomes a priority for a wider industry.

In the present paper, the authors are proposing an optional gettering method that would allow capturing uncontrolled impurity atoms in the silicon lattice (such as Fe, Cu, W), including oxygen $O_2$.

## 2. METHODOLOGY

The gettering properties of nickel clusters were studied in 3 different states, i.e., 1 – in original (reference) samples, 2 – in samples with additionally doped lattice site impurity atoms and 3 – in samples with additionally doped interstitial impurity atoms. Atoms of sulfur were chosen as additional dopants for lattice site impurity role whereas atoms of manganese as additional interstitial impurity atoms.

Single crystalline *p*– and *n*–type silicon wafers with resistivity $\rho = 1$, 10, 100 Ohm·sm and concentration of oxygen $N_{02} = 7 \times 10^{17}$ cm$^{-3}$ were chosen as reference samples (no additional doping with any impurity). The doping process was carried out from a pre-deposited Ni metal layer at a temperature of 1200°C for $t = 1$–5 hours. Later, the samples were cleaned chemically and mechanically. Shortly thereafter, the samples were polished for further diagnostics by using an INFRAM-I-type infrared microscope. The samples were exposed to infrared light from underneath whereas transparent infrared images were taken from the surface.

The starting material of p-type silicon with conductivity $\rho = 1$ Ohm·sm was doped with sulfur. The process of diffusion by impurity atoms of sulfur was carried out from the gas phase after clusters of nickel atoms have been formed in the earlier stages. Under identical conditions, the reference silicon sample without nickel atoms was later doped with sulfur atoms [12, 13].

A silicon sample of p-type conductivity with a resistivity $\rho = 3$ Ohm·sm was doped with manganese. The diffusion of Mn was carried out after nickel clusters have been formed in the earlier stages. The Mn-doped silicon, processed during low-temperature diffusion, was chosen as a reference sample [14].

Experimental results were gained on IKS-21, scanning electron microscope SEM (Oxford Instruments





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ZEISS EVOMA-10) and infrared microscope (INFRAM-I).

## 3. RESULT AND DISCUSSION

On Fig. 1 one can clearly see uniformly distributed black dots across the sample. To make sure that these black dots are clusters of nickel atoms, we had studied their composition on a scanning electron microscope using energy dispersive spectroscopy (Fig. 2, spectrum 34). The results of experiments show that the proportion of nickel is ~18%. It should be noted that other impurity atoms, such as Fe, Cu, and W, were also found in the cluster.

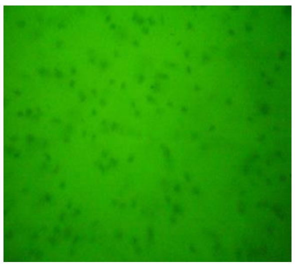

**Fig. 1** – An infrared image of silicon with nickel clusters

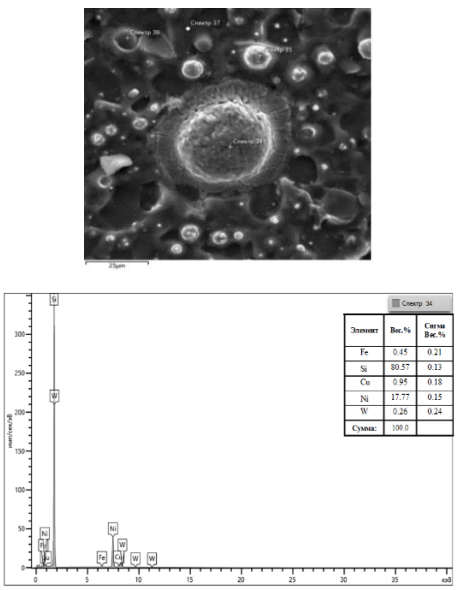


**Fig. 2** – Elemental analysis of a cluster at the “spectrum-34” point

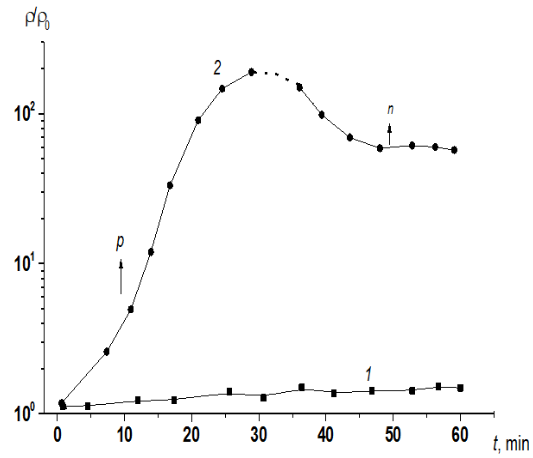


**Fig. 3** – Relative change in the resistivity of samples depending on the time of thermal annealing at T = 450°C, 1 – Si <Ni>, 2 – reference sample

Fig. 3 shows relative change in the resistivity of the samples depending on the time of additional annealing at a temperature of 450 °C. Reference samples of *p*-type conductivity with $\rho = 10$ Ohm·sm were annealed under similar conditions. As can be seen, the resistivity of samples with preformed nickel clusters practically do not change. At the same time, the resistivity of reference samples tends to increase as the thermal annealing time does increase and reaches its maximum value at $t = 30 \div 40$ min, where after the inversion of the conduction type occurs.

The above results once again confirm that the presence of nickel clusters (their electrically neutral portion) almost completely suppresses the generation of thermal donors, and the maximum concentration of thermal donors tends to manifest itself in the temperature range of 450 ÷ 500°C.

Table 1 shows key technological process parameters for nickel doping that ensure that initial electrical and recombination parameters of silicon would be retained, both in the process of nickel diffusion doping and during thermal annealing afterwards.

The above results were received while investigating the samples doped with nickel atoms. These studies prove that clusters of nickel atoms in the silicon lattice successfully suppress the activation of thermal donors.

**Table 1** – Key technological process parameters for nickel doping

| Parameters of reference silicon sample | | Temperature of diffusion of Ni | Duration of diffusion | After diffusion | After thermal annealing | | Temperature range of stability of parameters of initial samples | |
|---|---|---|---|---|---|---|---|---|
| TC | $\rho$, Ohm·sm | $T$, °C | $t$, min | $\rho$, Ohm·sm | $\rho$, Ohm·sm | $\tau$, μs | $T$, °C | $t$, hour |
| $n$ | ≤ 10 | 1100÷1150 | 15÷20 | 10 | 12 | does not change | 100÷700 | 1÷20 |
| $n$ | ≤ 40 | 1060÷1100 | 22÷25 | 42 | 45 | changes max 12% | 100÷600 | 1÷20 |
| $n$ | ≤ 100 | 1050 | 30÷35 | 95 | 102 | changes max 18% | 100÷500 | 1÷20 |
| $p$ | ≤ 10 | 1150÷1100 | 15÷20 | 9 | 11 | slightly changes | 100÷700 | 1÷20 |
| $p$ | ≤ 40 | 1100÷1050 | 20÷25 | 40 | 43 | changes 18÷20% | 100÷700 | 1÷20 |
| $p$ | ≤ 100 | 1050÷1000 | 30÷35 | 98 | 104 | changes 12÷15% | 100÷500 | 1÷20 |

This confirms that nickel clusters have gettering properties in the silicon lattice that would allow removing uncontrolled impurities that always exist in the crystal lattice. Further study of gettering properties of nickel clusters in removing other impurity atoms will be required [5, 15-18].

Moreover, the presence of clusters of impurity atoms of nickel in silicon pre-doped with sulfur makes it possible to extend the photosensitivity parameter and thus reveal other energy levels of sulfur in silicon.

The results of experimental studies are presented in Table 2. As the results show, the samples doped with nickel and sulfur nearly manifest the same parameters as the silicon doped only with sulfur. This shows that the presence of Ni atomic clusters has practically no effect on the state of sulfur atoms in silicon.

**Table 2** – The results of experimental studies

| No | Samples | $\rho$, Ohm·sm | $\mu$, cm$^2$/V·s | type | $N$, cm$^{-3}$ | $E$, eV | $F$, eV | $N_{AS}$, cm$^{-3}$ |
|---|---|---|---|---|---|---|---|---|
| 1 | Si (Ni) | 0.97 | 270 | $p$ | $2.50 \cdot 10^{15}$ | 0.22 | 0.17 | – |
| 2 | Si (S) | 9.9 | 1190 | $n$ | $5.50 \cdot 10^{14}$ | 0.24 | 0.27 | $4.3 \cdot 10^{15}$ |
| 3 | Si (Ni, S) | 10.8 | 1165 | $n$ | $4.87 \cdot 10^{14}$ | 0.30 | 0.27 | $4.2 \cdot 10^{15}$ |

Fig. 4 shows spectral dependences of photoconductivity of Si<S> and Si<Ni, S> samples measured under identical conditions. As can be seen from the figure, almost in all samples and in the entire investigated diapason of the spectrum, the photosensitivity of Si<Ni, S> samples is significantly higher than in Si<S> samples, this is especially starkly manifested in the range $h\nu = 0.5 \div 1.1$ eV

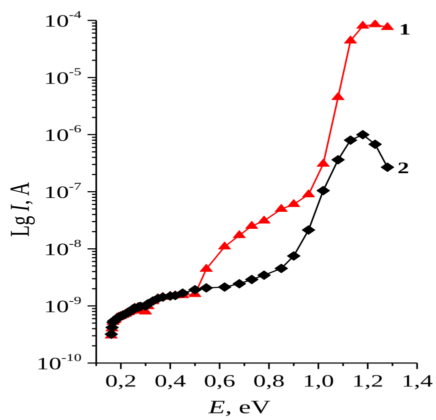


**Fig. 4** – Spectral dependence of the photoconductivity of samples at $T = 100$ K, 1 – Si<Ni, S>, 2 – Si<S>

This helps suggest that removing impurities from the silicon crystal lattice with nickel clusters makes it possible not only to increase the photosensitivity of Si<Ni, S> samples in the region of intrinsic absorption spectrum, but also to expand the photosensitivity towards longer wavelengths of infrared wavelengths $\lambda = 2.5 \div 11$ μm.

Fig. 5 shows the composition of these samples. Investigations on “Spectrum 27” showed the following results of elemental analysis: Si – 83 %, O – 8,8 %, S – 4.7 %, Ni – 3.4 %.

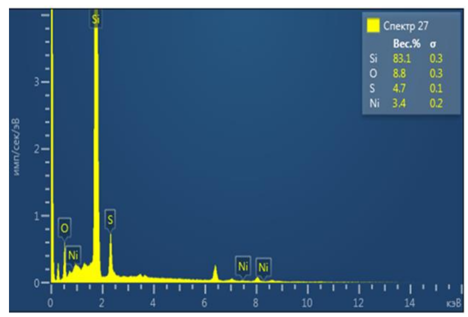


**Fig. 5** – The composition of nickel clusters on "Spectrum 27" determined using the method of energy dispersive X-ray spectroscopy EDS

The results of parameters of the samples are shown on Table 3. As can be seen from Table 3 in the investigated sample, the resistivity becomes almost an order of magnitude lower, and the photosensitivity of the material decreases significantly (almost 600 times). Additionally, the authors have also studied the spectral dependence of the photoconductivity of these samples (Fig. 6).

**Table 3** – Electrical parameters of samples after diffusion at $T = 1070$ °C

| Ref. sample | Impurity | type | $\rho$, Ohm·sm | $\mu$, V/cm·s | $N$, cm$^{-3}$ | $I/I_0$ |
|---|---|---|---|---|---|---|
| KDB-3 | Ni, Mn | $p$ | $1{,}5 \cdot 10^2$ | 330 | $1{,}8 \cdot 10^{14}$ | 9 times |
| | Mn | $p$ | $2{,}3 \cdot 10^3$ | 360 | $7 \cdot 10^{12}$ | 5530 times |

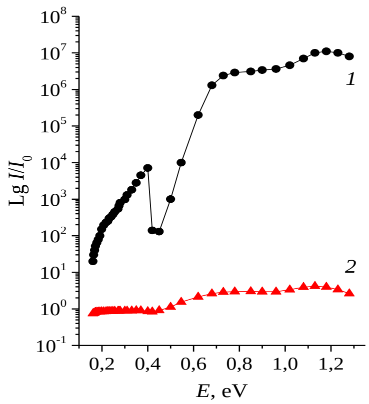


**Fig. 6** – Photospectral dependence of samples at $T$ = 100 K, 1 – Si<Mn>, 2 – Si<Ni, Mn>

The reference sample is characterized by high photosensitivity in the infrared region of 0.12 – 1.2 eV (Fig. 6, curve 1). At the same time, there is an effect of photoconductivity quenching, the minimum of which lays in the vicinity of 0.45 eV. In manganese-doped silicon samples with nickel clusters, a slight spectral sensitivity was revealed in the region of 0.5 – 1.2 eV (Fig. 6, curve 2). The experimental results show that the photoelectric properties of silicon samples with clusters of impurity atoms of nickel differ significantly from those in reference ones.

## 4. CONCLUSION

Based on the results of experimental studies, it has been established that, in contrast to the previously known methods of gettering and stabilizing the electrical and recombination parameters of silicon, nickel doping of silicon has the following main advantages:

– In times of diffusion doping of silicon with nickel, the initial electrical parameters (charge carrier concentration, mobility, resistivity) remain practically unchanged.

– In times of diffusion doping of silicon with nickel, lifetime of minority charge carriers does not virtually change (or if changes, so it does by a maximum of 12 ÷ 18 % of its original value), which would not be possible to attain with other gettering methods.

The nickel-doped silicon material with certain initial properties and under certain diffusion conditions retains its electrical parameters and minority charge carrier lifetime during subsequent heat treatments at T = 100 ÷ 700 °C for a comparatively long time ($t$ = 1 ÷ 20 hours).

Thus, on the basis of the above experimental results, it can be justified that, by forming nickel clusters in the silicon crystal lattice, it becomes possible to remove the existing fast-diffusing impurities in the silicon lattice, earlier doped site and interstitial impurities, as well as oxygen atoms that stimulate generation of recombination centers and thermal defects.

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## Кластери нікелю в решітці кремнію

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Досліджено гетерні властивості кластерів нікелю в решітці кремнію. Досліджено гетеруючі властивості кластерів нікелю в різних станах, тобто у вихідних (еталонних) зразках, а також у зразках з додатково легованими домішковими атомами сірки та марганцю між вузлами та вузлами ґратки. Електрофізичні та фотоелектричні параметри досліджували за допомогою сучасної апаратури: інфрачервоного мікроскопа типу INFRAM-I, IKS-21 та скануючого електронного мікроскопа SEM (Oxford Instruments ZEISS EVOMA10), IKS-21. Також запропоновано нову технологію, що дозволяє отримувати шкідливі домішки; рекомендовано для широкого застосування в електронній промисловості та науково-дослідних інститутах для виробництва матеріалів зі стабільними параметрами та розробки принципово нових пристроїв.

**Ключові слова**: Кремній, Нікель, Кластер, Теплові донори, Температура, Дифузія, Час життя.