

ELECTROPHYSICAL PROPERTIES OF SILICON DOPED WITH LUTETIUM

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Abstract. This article discusses the electrical properties of silicon doped with lutetium. The diffusion method is used in the fabrication of silicon structures doped with lutetium. n-Si, p-Si, n-Si<Lu> and p-Si<Lu> were prepared to measure electrophysical parameters. The resistivity of the samples, the mobility of charge carriers, the concentration and the distribution of electrophysical parameters depending on the temperature and thickness of the sample have been studied. These parameters were determined by the four-probe van der Pauw method. Research work was carried out at room temperature and in the range of 77÷300 K. Ohmic contact was obtained through a mixture of 1% Sb + 99% Au for measuring samples on the HMS500 instrument. The resistivity and concentration of charge carriers were also studied, taken from a distance of 2 μm from the surface of the samples. The electrical parameters of the samples were measured using an Ecopia Hall effect measurement system. The electrical parameters of the p-Si and p-Si<Lu> samples did not change significantly. Changes in the surface morphology of these samples were observed in the results obtained in ACM.

Keywords: Silicon, lutetium, diffusion, resistivity, concentration, mobility, Hall effect, four probes.

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1. Introduction

Today, the rapid development of science and technology requires the creation of semiconductor devices that are compact, resistant to external influences and have high sensitivity. A lot of scientific work is being done on the formation of a deep energy level in silicon, which is the main material of semiconductor devices, doping with inputs that allow changing its properties, as well as studying the thermal and radiation effects on them (Daliev *et al.*, 2023; Abdurakhmanov *et al.*, 1998; Utamuradova *et al.*, 2023; Azamatov *et al.*, 2023).

The growing role of modern electronics in scientific and technological development leads to an increase in the requirements for the reliability of semiconductor devices. One

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of the main ways to solve this problem is to obtain and improve semiconductor materials with special properties.

The field of application of solid-state devices is constantly expanding, fundamentally new devices are being created that stimulate the development of industry in new directions, which requires a significant increase in the perfection of the structure of Si, the main material of modern semiconductor solid-state electronics. In this regard, studies aimed at studying the processes of defect formation in Si doped with various impurities and establishing controlled methods for stabilizing the parameters of semiconductor devices are one of the important problems.

Electronic processes in semiconductor materials are determined mainly by bulk and surface defects of the semiconductor. The study of these defects and the reduction of their formation is one of the main tasks of modern semiconductor electronics. In recent years, there has been a significant increase in interest in the development of methods for controlling defects in silicon single crystals and their interaction by doping with rare earth elements (REE) (Utamuradova *et al.*, 2006; Brinkevich *et al.*, 2002). An analysis of the results of many studies shows that the inclusion of rare earth elements in silicon significantly affects the process of formation of thermal and radiation defects in it, without exhibiting electrical activity. Until now, the nature of REE incorporation into silicon has not been comprehensively studied and the available results have a contradictory description. The main advantage of REE is determined, first of all, by the fact that they do not show electrical activity immediately after the growth of a single crystal. However, they can have a significant effect on the processes of defect formation and on the state of the defect-impurity ensemble of the crystal as a whole. Research carried out in this direction is mainly aimed at solving the problems of increasing the thermal and radiation resistance of semiconductors, obtaining materials with precisely controlled properties, as well as studying the processes of interaction of rare earth elements with technological compounds in silicon (Daliev *et al.*, 2023; Bahadyrkhanov *et al.*, 2011; Utamuradova *et al.*, 2023; Daliev *et al.*, 2021).

2. Experimental part

Silicon structures based on rare earth elements were obtained by the diffusion method. The single crystals of silicon of n-type ($\rho=0.3\div150\ \Omega\cdot\text{cm}$) and p-type ($\rho=0.3\div20\ \Omega\cdot\text{cm}$) grown by Czochralski method were used for research (Anfimov *et al.*, 2007). At the input, the element lutetium was obtained with a purity of 99.999%.

Before diffusion, silicon single crystals were subjected to mechanical and chemical treatment. Lutetium atoms were deposited onto the surface of a silicon sample using a VUP-4 setup under high vacuum conditions ($10^{-6}\ \text{mm Hg}$). A high vacuum ampoule was obtained using quartz glass. Diffusion was carried out in a SOUL oven at a temperature of 1523 K for 30 hours. After diffusion, the samples were rapidly cooled. The thin oxide layer formed on the surface of the silicon sample was removed using the CP-4 mixture. After diffusion annealing, the samples were rapidly cooled. An ohmic contact was obtained using a mixture of 1% Sb + 99% Au to measure the electrophysical parameters of the samples on the HMS500 instrument.

After diffusion, the resistivity of the Si<Lu> samples was measured by the four-probe method. The resistivity of n-Si<Lu> samples varied from $35.5\ \Omega\cdot\text{cm}$ to $5383\ \Omega\cdot\text{cm}$. In p-Si<Lu> samples, the resistivity value did not change. The conductivity type of the samples was determined using a thermal probe; according to the results obtained, after

diffusion, a change in the conductivity type of the n-type samples to the p-type was observed.

3. Results and their discussion

Currently, special importance is attached to the study of the nature of collections of rare earth elements introduced into semiconductor single crystals by the diffusion method. An estimate of the co-concentration of electroactive REE ions in the upper layer of silicon, data from measurements of the mobility of charge carriers by the Hall method, as well as results from measuring the resistivity of the sample using the four-probe method were obtained. Doping silicon with lutetium led to the appearance of acceptor centers. The fact that the content of the element lutetium from 0.03 to 1.8 mass percent changes the type of conductivity of the sample, but does not change the concentration of holes in silicon, was established by the methods of the Hall effect and electrical conductivity. The profile was determined by thin film deposition (in 1HF:50HNO₃ solution) and measurement of the surface resistance of the sample by the four-probe method, as well as by the Hall effect method using the Van der Pauw method (Askerov *et al.*, 2020; Wang *et al.*, 2006).

The charge carrier concentration $p(x)$ is determined by the following formula.

$$p(x) = \frac{1}{e} \frac{\left(\frac{d\sigma_s}{dx}\right)^2}{\frac{d}{dx}(R_s \sigma_s^2)}$$

Here is R_s the measured (effective) Hall coefficient, σ_s is the surface conductivity and e is the electronic charge. Removable layer thickness 523-142, measured at MITUTOYO. As in the study of other rare earth elements impurities in silicon, electrical measurements, as well as atomic force microscopy, performed at several points on the surface, showed that the lutetium impurities were unevenly distributed in the cross-section of the sample. Atomic force microscopy, carried out before and after washing, as well as during the process of removing layers, showed a uniform distribution of lutetium impurities and the absence of inclusions in the cross section of the sample.

The resistivity of the sample was measured using the HMS500 instrument. The relative resistance of a KEF-40 silicon single crystal in the initial state and silicon single crystal samples (control) thermally annealed at 1523 K for 30 hours were also measured. There were no changes in the depth distribution of resistivity of n-Si and n-Si (control) samples. It was observed that the resistivity of the n-Si<Lu> samples remained virtually unchanged after 80 μm . It has been established that the change in resistivity of lutetium-doped silicon samples depends on the diffusion time and diffusion temperature.

As can be seen from Figure 1, the resistivity values of n-Si and n-Si (control) are almost close to each other. It can be seen that the resistivity of the lutetium-doped silicon single crystal increased sharply; as the sample surface moved away from the thickness of 2 μm , the resistivity value decreased to 80 μm . The results obtained show that the resistivity of n-Si<Lu> samples doped with lutetium increases from 40 $\Omega\cdot\text{cm}$ to $5.5\cdot 10^3$ $\Omega\cdot\text{cm}$ and the resistivity of p-Si<Lu> samples practically does not change. Thus, the resistivity distribution of lutetium-doped n-type silicon samples decreased to 80 μm and then stabilized. The studies were carried out on samples of different brands and resistivity 0.3÷150 $\Omega\cdot\text{cm}$.

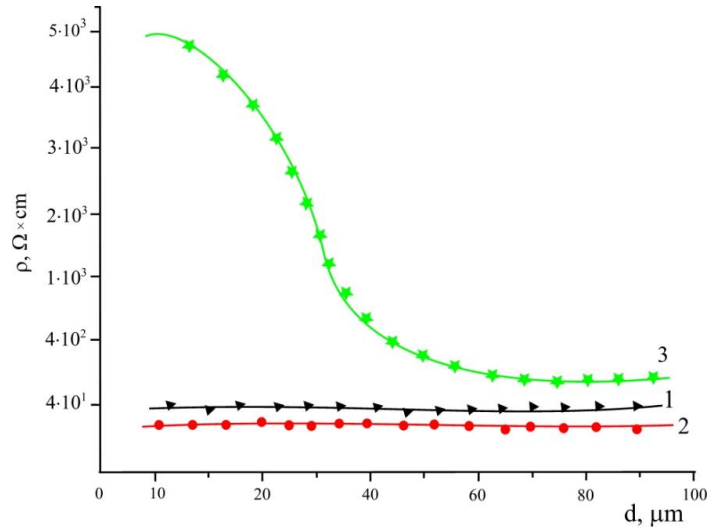


Figure 1. Resistivity distribution over thickness at room temperature.
1-n-Si; 2-n-Si (control); 3-n-Si<Lu>

The experiment revealed that the electrical parameters of samples of n- and p-type silicon single crystals doped with lutetium with low relative resistance do not change. Based on the results obtained, it was experimentally established for the first time that the nature of lutetium atoms in silicon is acceptor. The results of these studies show that all n-type samples doped with lutetium undergo a change in conductivity type and a sharp change in resistivity. For p-type samples, in this case, the value of resistivity somewhat decreases, while the type of conductivity remains unchanged.

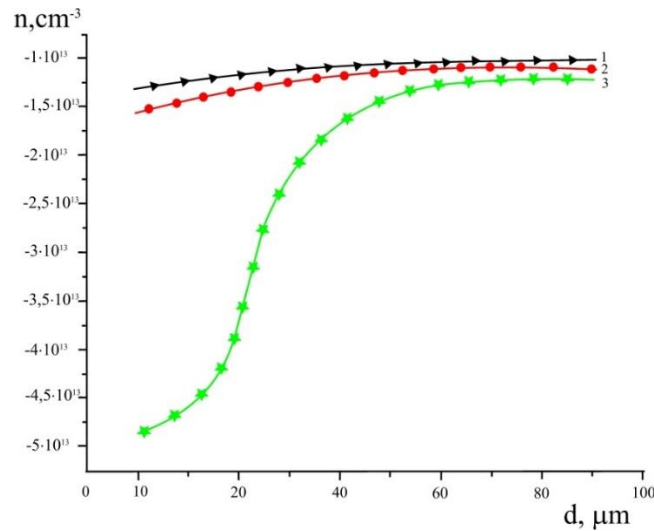


Figure 2. The distribution of the concentrations of the main charge carriers over the thickness at room temperature. n-Si; 2-n-Si (control); 3-n-Si<Lu>

In Figure 2 shows the distribution of the concentration of the main charge carriers over the thickness. The concentration of major charge carriers HMS500 was measured from the surface of n-Si, n-Si (control) samples taken from 2 μm . As can be seen from the figure, the concentration of the main charge carriers decreases in the sample doped with lutetium. This situation was not observed in the n-Si and n-Si samples (control). Thus, most lutetium atoms in silicon are electrically neutral and centers are formed in which electrically neutral lutetium atoms hold charged defects in the bulk of silicon. The formation of such centers in silicon doped with rare earth elements has been confirmed by a number of studies. Some of the diffusing REE ions interact with thermal donors generated at high temperature and these complexes facilitate the diffusion of charge carriers. For all studied REEs, the hole concentration lies within the range of 10^{14} and 10^{17} cm^{-3} , that is, the elements are less than their co-concentrations. The mobility of free charge carriers depends on the properties of the crystal lattice, access to it and temperature. The reason for this is the process of charge carrier scattering. The works examined the scattering of conduction electrons and holes on neutral atoms and impurity ions in a crystal on point defects in the structure, dislocations and thermal fluctuations of the lattice.

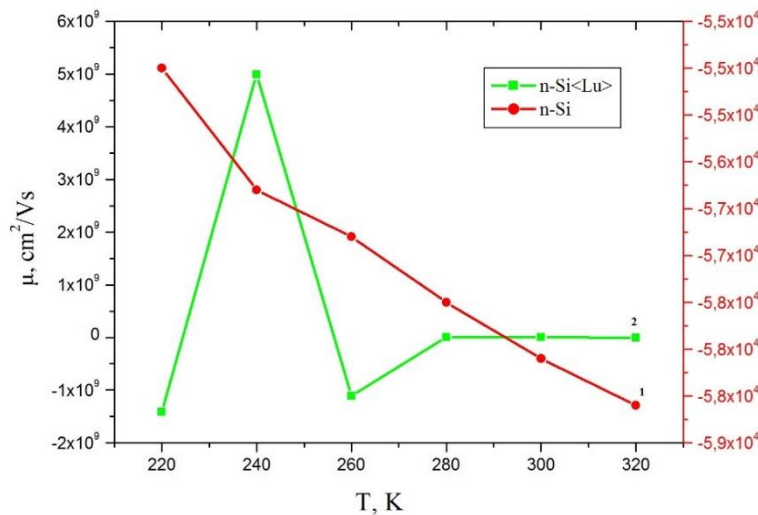


Figure 3. Mobility distribution of the majority charge carriers as a function of temperature. 1-n-Si (control); 2-n-Si<Lu>

In Figure 3 shows the change in the mobility of the main charge carriers in the range of 220÷320 K. n-Si (control) sample changed to $-5.5 \cdot 10^4 \div 5.9 \cdot 10^4 \text{ cm}^2/\text{Vs}$ in the temperature range 220÷320 K. n-Si<Lu> sample changed to $-1.38 \cdot 10^9 \div 5 \cdot 10^9 \text{ cm}^2/\text{Vs}$ in the temperature range 220÷240 K, $5 \cdot 10^9 \div -1.1 \cdot 10^9 \text{ cm}^2/\text{Vs}$, in the temperature range 240÷260 K. It changed to changed to $-1.1 \cdot 10^9 \div 6 \cdot 10^5 \text{ cm}^2/\text{Vs}$ in the temperature range 260÷320 K.

Such an unstable change in mobility is usually observed in rare earth elements. This convincingly indicates that the crystal lattice of doped silicon with lutetium inclusions is strongly distorted due to large differences between the radii of silicon and lutetium ions. The ionic radius of the tetravalent silicon ion is 42 pm, while the radius of the trivalent lutetium ion ranges from 81 to 122 pm for lanthanum. The exchange of silicon for lutetium at the site of the crystal lattice causes its deformation and this leads to the

formation of specific point defects, which serve as additional diffusion centers around the exchange ion.

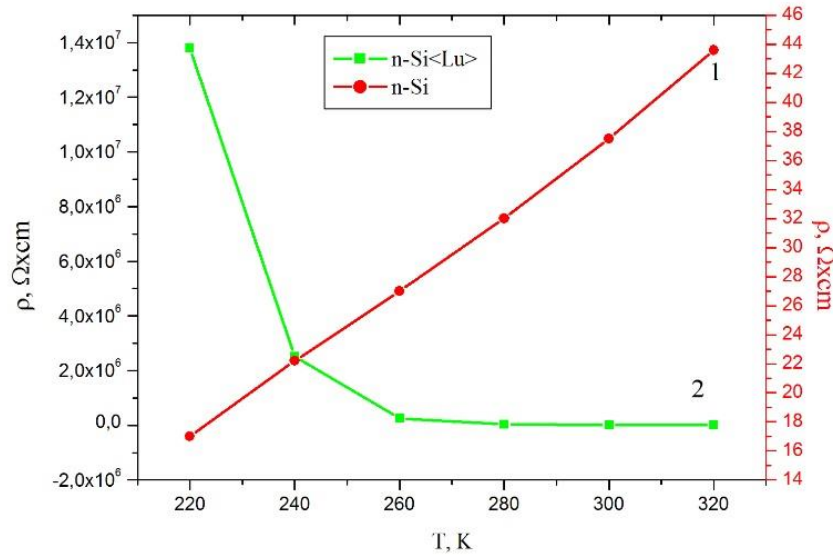


Figure 4. Relative resistance distribution as a function of temperature.
1-n-Si (control); 2-n-Si<Lu>

A sharp increase in resistivity was observed in silicon samples doped with most rare earth elements. In particular, such a process was observed in our research work. As can be seen from Figure 2, the resistivity of the n-Si sample (control) varies from 17 Ω·cm to 43.6 Ω·cm in the temperature range 220÷320 K.

the n-Si<Lu> sample increased and the HMS500 exceeded the measurement limit due to the increase in temperature to the resistivity measurement limit. The relative resistance decreased exponentially from $1.38 \cdot 10^7$ Ω·cm to $3.78 \cdot 10^3$ Ω·cm in the temperature range 220÷320 K.

In this case, the surface concentration of lutetium atoms in silicon, determined using the labeled atom method, is $\sim 5,3 \cdot 10^{13}$ cm⁻³. As the analysis of the data obtained shows, the diffusion coefficients and activation energies of lutetium in silicon are in the range of values characteristic of the diffusion of typical group III elements as well as for other rare earth elements that are substitutional impurities and diffuse over the sites of the crystal lattice. This allows us to assert that lutetium, elements of the same group, are also substitutional impurities and diffuse like other rare earth elements along the sites of the silicon crystal lattice. A comparison of the latest data with early indicators of the diffusion of rare earth elements in silicon, obtained using radioactive and other techniques, shows that the method of applying the diffusant and the diffusion medium do not significantly affect the diffusion parameters of rare earth elements in silicon.

4. Conclusion

Based on the analysis of the research results, the following conclusions can be drawn:

When an n-type silicon single crystal was doped with lutetium, a change in the type of conductivity and a sharp increase in resistivity were found. When doping single crystals of p-type silicon (p-Si) with lutetium (p-Si<Lu>), for the first time in scientific research, a slight change in resistivity and no change in the type of conductivity was observed.

In silicon samples doped with lutetium and heat-treated by the diffusion method, the resistivity measured over the depth (thickness) of the sample shows a sharp increase in r in the initial part up to a depth of $\sim 80 \mu\text{m}$, then the value of r stabilizes and there is no significant change in r over the thickness of the sample.

It has been established that the mobility of charge carriers in the temperature range $220\div 320 \text{ K}$, the unstable change in the mobility of the n-Si<Lu> sample, the exchange of silicon for lutetium at the junction of the crystal lattice cause it to deform and this leads to the formation of specific point defects that serve as additional diffusion centers around the exchange ion.

It was found that the resistivity of n-Si<Lu> samples decreases exponentially from $1.38 \cdot 10^7 \Omega \cdot \text{cm}$ to $3.78 \cdot 10^3 \Omega \cdot \text{cm}$ in the temperature range $220\div 320 \text{ K}$.

The nature of lutetium atoms in silicon is of an acceptor nature; it has been established experimentally for the first time.

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