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REGULAR ARTICLE

Influence of Accumulation of Impurity Atoms Ni and Fe on the Electrophysical Properties of Si Single Crystals

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The article discusses the processes of formation of impurity accumulations in silicon, simultaneously doped with impurity atoms of nickel and iron at a temperature of $T = 1473$ K. The structural structures and elemental composition of impurity accumulations, which have different morphological parameters, are studied. The results of structural analyzes showed that the formation of any massive accumulations of impurity atoms was not observed in the volume of the initial samples. Unlike the original samples, in the volume of n-Si<Ni, Fe> samples, the formation of accumulations of impurity atoms of various geometric shapes is observed, the sizes of which reach up to several hundred nanometers. It has been revealed that in the volume of impurity accumulations, in addition to atoms of the matrix element silicon and the main impurities of nickel and iron, there are also atoms of so-called technological impurities such as carbon and oxygen. Analyzes of the chemical composition of an impurity accumulation with a spherical shape, the diameter of which is 400 nm, showed that in the central region of this impurity accumulation the percentage of impurity Ni atoms is 30.76 %, and iron atoms are 16.34 %. Also presented are the results of studies of the effect of thermal annealing on the resistivity of n-Si<Ni, Fe> samples at temperatures $T = 673 \div 1273$ K in a time interval of $10 \div 120$ minutes, followed by sharp quenching. As it turned out, in the dependences of the relative resistivity of n-Si<Ni, Fe> samples on the duration of the annealing time, a certain tendency is observed, according to which, with increasing annealing temperature, the maximum in the dependence curves occurs at a shorter annealing time. Using electron microscopy, structural analyzes of the state of impurity accumulations before and after exposure to thermal annealing were carried out.

Keywords: Morphology, Accumulations, Silicon, Nickel, Iron, Decomposition.

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1. INTRODUCTION

It is known that impurity defects formed during high-temperature diffusion doping of single-crystal silicon with elements of 3d transition metals significantly affect their electrical properties. In this direction, special attention is drawn to the study of the morphological parameters of impurity micro- and nanoinclusions formed on the surface and in the bulk of silicon, as well as their behavior under the influence of external influences [1-4]. In addition, the state and behavior of accumulations of impurity atoms of transition metals under the influence of external impacts (temperature, pressure, irradiation) is of great scientific and practical interest from the point of view of controlling the electrical properties of silicon single crystals [5-7]. In this regard, this paper presents the results of studies of the morphological parameters of impurity accumulations formed in the bulk of silicon, as well as the effect of thermal treatment on the resistivity of silicon doped with nickel and iron.

2. DESCRIPTION OF THE OBJECT AND RESEARCH METHODS

Samples n-Si<Ni, Fe> samples obtained from the starting material – single-crystalline silicon, with a resistivity of $\rho = 40$ Ohm·cm, grown by the Czochralski method were chosen as research objects. The samples had the shape of a parallelepiped with corresponding dimensions of 2 × 5 × 10 mm. Simultaneous diffusion of nickel and iron in silicon was carried out at a temperature of 1473 K for 4 hours. After diffusion annealing, the samples were cooled at a rate of 0.05 K/s. The resulting n-Si<Ni, Fe> samples, in place with the original n-Siorig samples, were subjected to isothermal treatment at temperatures $T = 673 \div 1273$ K in a time interval of $10 \div 120$ minutes, followed by sharp quenching. After each annealing stage, the electrical properties of the samples were studied. The resistivity of the samples was measured using the Hall effect method on an Ecopia HMS-7000 instrument. Structural studies were carried out by scanning electron microscopy using a modern JSM-IT200 SEM installation, which allows one to obtain enlarged images of impurity accumulations formed in solid crystals and conduct an elemental analysis of their composition. The modern computer microscope control system is very simple; all control func-

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tions are automated. In addition to the standard high vacuum mode, the device has a mode for measuring samples under controlled low vacuum conditions. The electron accelerating voltage in our case was 20 kV, while the pressure in the sample chamber was 80 Pa.

3. DESCRIPTION AND ANALYSIS OF RESULTS

Using a JSM-IT200 scanning electron microscope, we carried out comprehensive studies of the structure of n-Si and *n*-Si<Ni, Fe> samples. Structural analyzes of these samples showed that, unlike the original samples, clusters of impurity atoms are formed in *n*-Si<Ni, Fe> samples. Fig. 1 shows a snapshot of the original sample, in the volume of which the formation of any massive clusters is not observed. In the volume of *n*-Si<Ni, Fe> samples, the formation of accumulations of impurity atoms of various geometric shapes is observed, the dimensions of which reach several hundred nanometers (Fig. 2).

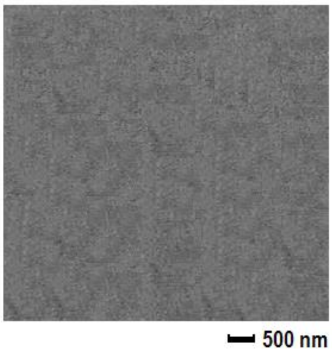

Fig. 1 – The photo of the original *n*-Si sample obtained using a JSM-IT200 SEM setup

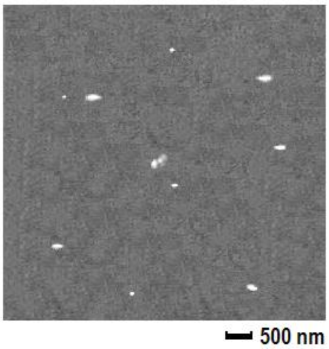

Fig. 2 – The photo of an *n*-Si<Ni, Fe> sample obtained using a JSM-IT200 SEM setup

The results of structural analyzes obtained with *n*-Si<Ni, Fe> samples showed that impurity clusters with various geometric shapes are formed in their volume, the sizes of which reach up to ~ 500 nm. In Fig. 3 shows the result of an analysis of the elemental composition of an impurity cluster with a spherical shape, the diameter of which is 400 nm, formed in the *n*-Si<Ni, Fe> sample. As can be seen, in the volume of the impurity accumulation, in addition to silicon atoms and the main impurities of nickel and iron, there are also atoms of so-called technological impurities, such as carbon and oxygen. The results of the analysis of the chemical composition showed that in the central region of this impurity accumulation the percentage of silicon atoms is 51.82 %. And for atoms of basic and technological impurities, this indicator has the following values: Ni atoms – 30.76 %, iron atoms – 16.34 %, oxygen atoms – 0.65 % and carbon atoms – 0.43 %.

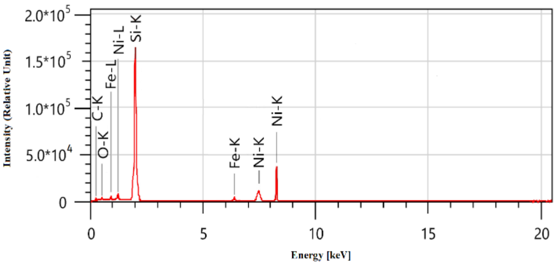

Fig. 3 – Full spectrum of the elemental composition of an impurity cluster with a spherical shape with a diameter of 400 nm, formed in the *n*-Si<Ni, Fe> sample

The results of studies of the dependence of ρ/ρ_0 on annealing time in *n*-Si<Ni, Fe> samples with a resistivity of $\rho = 2\cdot10^3$ Ohm·cm showed that during heat treatment at a temperature of 673 K there were no significant changes in the value of ρ samples observed (curve 1, Fig. 4). In the subsequent heat treatment at $T = 873$ K for 30 minutes, the value of ρ/ρ_0 of the samples remains almost unchanged (curve 2, Fig. 4). With a further increase in time to 40 minutes, a significant increase in the ρ value of the samples is observed, where it increases by ~ 40 % and reaches its maximum. During the subsequent increase in annealing time to 120 minutes, the value of ρ/ρ_0 of the samples gradually decreases and reaches almost its original value.

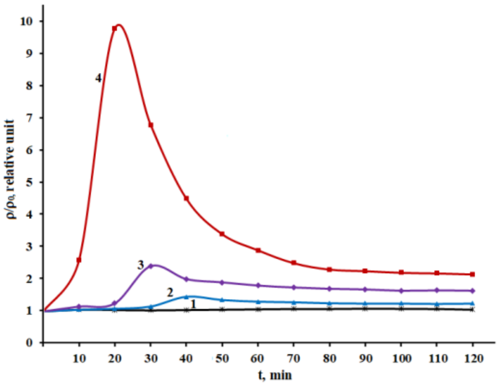

Fig. 4 – Dependences of ρ/ρ_0 values on annealing time in *n*-Si<Ni, Fe> samples at temperatures: 1 – 673 K; 2 – 873 K; 3 – 1073 K; 4 – 1273 K

At the thermal annealing temperature $T = 1073$ K for 20 minutes, a slight increase is observed in the value ρ/ρ_0 of *n*-Si<Ni, Fe> samples, which is ~ 20 % (curve 3, Fig. 4). A further increase in the annealing time to 30 minutes leads to a sharp increase in the value of ρ/ρ_0 of the samples by almost 2.5 times. In subsequent annealing times, it begins to gradually decrease and at 120 minutes the value of $\rho$is equals to $2{,}4\cdot10^3$ Ohm·cm.

In the obtained results of the dependence of ρ/ρ_0 on the annealing time at $T = 1273$ K, a more significant increase in the value of the resistivity of *n*-Si<Ni, Fe>

samples is observed. Annealing at this temperature for 20 minutes leads to a sharp increase in the value of ρ/ρ_0 samples by almost one order of magnitude (curve 4, Fig. 4). After which a sharp decrease in this value is observed and upon reaching 50 minutes, the value of the resistivity of the samples is $\rho = 6.4 \cdot 10^3$ Ohm·cm. With a further increase in the annealing time to 120 minutes, it continues to slowly decrease and reaches the value $\rho = 4.5 \cdot 10^3$ Ohm·cm. It should be noted that in the dependences of ρ/ρ_0 values on time, in n-Si<Ni, Fe> samples there is a certain tendency, according to which, with increasing thermal annealing temperature, the maximum in the dependence curves occurs at a shorter annealing time.

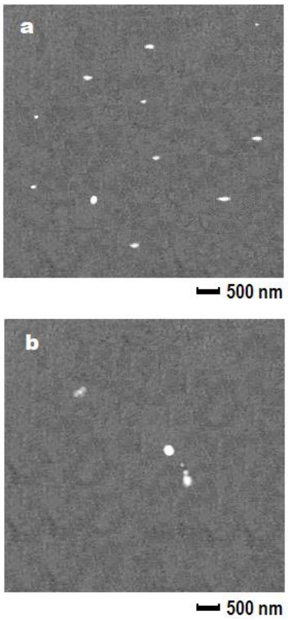

Fig. 5 – Photos of impurity nanoclusters in n-Si<Ni, Fe> samples before (a) and after (b) heat treatment at $T = 1273$ K

In order to clarify the physical nature of such changes in the dependences of ρ/ρ_0 values on annealing time in n-Si<Ni, Fe> samples, we carried out additional studies to study the state of impurity accumulations before and after exposure to thermal annealing. The results of analyzes of n-Si<Ni, Fe> samples before and after annealing at $T = 1273$ K showed that under the influence of annealing, the density of impurity nanoclusters up to 400 nm in size sharply decreases (Fig. 5). The obtained photographs show that, under the influence of thermal annealing, impurity accumulations disintegrate.

4. CONCLUSIONS

Thus, based on the results obtained, it has been established that with simultaneous diffusion doping of silicon with nickel and iron impurities at $T = 1473$ K for 5 hours, various accumulations of impurity atoms are formed. The sizes of these clusters reach up to several hundred nanometers and they have different geometric shapes. It was also revealed that the volume of impurity accumulations contains atoms of silicon, nickel, iron, as well as atoms of technological impurities such as carbon and oxygen. It was determined that under the influence of thermal annealing at $T = 1273$ K for 20 minutes, impurity accumulations with sizes up to 400 nm disintegrate.

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REFERENCES

1. A. Haarahiltunen, M. Yli-Koski, H. Savin, *Energy Procedia* 8, 355 (2011).
2. S.Z. Zainabidinov, K.N. Musaev, N.A. Turgunov, A.R. Turaev, *Inorgan. Mater.* **48**, 1065 (2012).
3. Sh.B. Utamuradova, Kh.S. Daliev, Sh.Kh. Daliev, K.M. Fayzullaev, *Appl. Phys.* **6**, 90 (2019).
4. Ch. Sun, H.T. Nguyen, F.E. Rougieux, D. Macdonald, *J. Crystal Growth.* **460**, 98 (2017).
5. N.A. Turgunov, E.Kh. Berkinov, D.X. Mamajonova, *J. Nano-Electron. Phys.* **13** No 5, 05006 (2021).
6. M.V. Trushin, O.F. Vyvenko, M. Seibt, *Solid State Phenomena* **131-133**, 155 (2008).
7. Ph. Saring, M. Seibt, *Phys. Status Solidi B* **258**, 2100142 (2021).
8. S.Z. Zainabidinov, N.A. Turgunov, *Russ. Phys. J.* **47** No 12, 1307 (2004).
9. N.A. Turgunov, E.Kh. Berkinov, R.M. Turmanova, *E3S Web of Conferences* **402**, 14018 (2023).
10. N.A. Turgunov, *Inorgan. Mater.* **54** No 12, 1183 (2018).
11. N.A. Turgunov, E.Kh. Berkinov, R.M. Turmanova, *Am. J. Appl. Sci. Technol.* **03**, 53 (2023).
12. N.A. Turgunov, E.Kh. Berkinov, D.Kh. Mamajonova, *Appl. Phys.* No 3, 40 (2020).
13. M.K. Bakhadyrkhanov, Kh.M. Iliev, K.S. Ayupov, B.A. Abdurakhmonov, Yu.P. Krivenko, R.L. Kholmukhamedov, *Inorgan. Mater.* **47** No 9, 962 (2011).
14. N. Turgunov, S. Zainabidinov, E. Berkinov, Sh. Akbarov, *Euroasian Journal of Semiconductors Science and Engineering.* **2** No 5, 19 (2020).

Вплив накопичення домішкових атомів Ni та Fe на електрофізичні властивості монокристалів Si

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У статті розглянуто процеси утворення домішкових скупчень у кремнії, одночасно легованому домішковими атомами нікелю та заліза при температурі $T = 1473$ K. Досліджено структурну структуру та елементний склад домішкових скупчень, які мають різні морфологічні параметри. Результати структурних аналізів показали, що в об'ємі вихідних зразків утворення будь-яких масивних скупчень домішкових атомів не спостерігалося. На відміну від вихідних зразків, в об'ємі зразків n-Si<Ni,Fe> спостерігається утворення скупчень домішкових атомів різної геометричної форми, розміри яких досягають кількох сотень нанометрів. Виявлено, що в обсязі скупчень домішок, крім атомів матричного елемента кремнію та основних домішок нікелю та заліза, присутні також атоми так званих технологічних домішок, таких як вуглець і кисень. Аналіз хімічного складу домішкового скупчення сферичної форми, діаметр якого становить 400 нм, показав, що в центральній області цього домішкового скупчення частка домішкових атомів Ni становить 30,76 %, а атомів заліза – 16,34 %. Також наведено результати досліджень впливу термічного відпалу на питомий опір зразків *n*-Si<Ni, Fe> при температурах $T = 673$-1273 K в інтервалі часу 10-120 хвилин з наступним різким гартом. Як виявилося, в залежностях відносного питомого опору зразків *n*-Si<Ni, Fe> від тривалості часу відпалу спостерігається певна тенденція, згідно з якою зі збільшенням температури відпалу максимум на залежності кривих відбувається за менший час відпалу. За допомогою електронної мікроскопії проведено структурний аналіз стану скупчень домішок до та після термічного відпалу.

Ключові слова: Морфологія, Кремній, Нікель, Залізо, Накопичення домішок.