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INFLUENCE OF DIFFUSION PARAMETERS ON THE MORPHOLOGY OF COBALT IMPURITY CLUMPS IN SILICON.

Sirojiddin .Z. Zainabidinov[1], Nozimjon.A. Turgunov[2], Shuhratjon.K. Akbarov[1]
[1]Andijan State University
[2]Research Institute of Physics of Semiconductors and Microelectronics at the National University of Uzbekistan
E-mail:shuhratjonakbarov31@gmail.com
E-mail: tna_1975@mail.ru

Abstract. The article examines the sequence of processes of formation of clusters of impurity cobalt atoms located in the volume of silicon single crystals in an electrically neutral state. The results of studies to determine the morphological parameters of impurity accumulations are presented. Based on the experimental data obtained, it was revealed that, depending on the size and shape of impurity accumulations, they have different structural structures. It has also been established that the atoms of the main and technological impurities have an uneven distribution over the volume of impurity accumulations.

Keywords: diffusion, impurity, silicon, cobalt, nickel, accumulation, morphology.

Introduction

Currently, the properties of impurity defects formed in the bulk of silicon single crystals doped with 3d metal impurities are being studied quite intensively. In previous studies in this area, the mechanisms of formation of impurity defects and their properties, and the diffusion parameters of atoms of 3d metal elements have been studied in sufficient detail. As well as the thermodynamic states of impurity defects in the bulk of silicon, the processes of formation and decay of impurity accumulations under the influence of external influences. It has been shown that among the transition 3d group metals, nickel, cobalt and copper have the highest diffusion and solubility coefficients in silicon. It has been experimentally established that with high-temperature doping of silicon with these impurities, the formation of complexes, clusters and precipitates, micro- and nano-accumulations in the bulk of silicon is observed. The electrical, photoelectric, optical and mechanical properties of semiconductor silicon with impurity clusters have been studied.

The results of electron microscopic studies of nickel-doped silicon samples carried out by the authors of [1, 2] showed that the forming impurity precipitates consist of several bands of varying contrast. The lightest area located in the center of the precipitate is identified by the authors as the metal phase. Based on the research results, the authors of [3] proposed a schematic model of nickel precipitate in silicon, according to which the central part, i.e. the core of the precipitate consists of metallic Ni, then silicides are deposited towards the surface of the precipitate in the order of decreasing proportion of Ni atoms in them.

The authors of works [4,5] used X-ray microprobing to study the mechanisms of formation and morphology of multicomponent metal particles in silicon doped with cobalt at low temperatures T<655 °C and high temperatures T>1200 °C. It has

been revealed that during high-temperature diffusion alloying followed by slow cooling, large intermetallic phases with sizes up to several microns are formed. The sizes and shapes of the forming particles were determined, as well as the dependence of the parameters of cobalt particles on the diffusion temperature and on the cooling rate of the samples.

The behavior of impurity atoms during the formation of impurity defects is important in the kinetics of the formation of various impurity clusters. The research results [6,7] showed that during diffusion doping, electroactive atoms of uncontrolled impurities will actively interact with atoms of the main impurity and form various clusters, which can be in thermodynamic equilibrium and nonequilibrium states. The state of impurity accumulations mainly depends on the diffusion parameters and the cooling rate of the samples after diffusion annealing [8].

Experimental technique

To study the sequence of processes involved in the formation of impurity clusters and their morphological parameters during diffusion doping, comprehensive investigations of the structure of single-crystal silicon doped with cobalt were carried out using electron probe microanalysis. The n-Si<Co> samples were obtained based on n-type single-crystal silicon with a specific resistivity of ρ=20 Ω·cm, grown by the Czochralski method. Cobalt diffusion in silicon was performed at a temperature of 1523 K for 2 hours. For the p-Si<Co> samples, n-type single-crystal silicon with a specific resistivity of ρ=40 Ω·cm was used. In this case, cobalt diffusion in silicon was carried out at a temperature of 1523 K for 4 hours, after which the samples acquired p-type conductivity. After diffusion, the samples were cooled at different cooling rates (υ_{cool} = 1÷400 K/s). The obtained samples underwent mechanical grinding to remove residual Co from the surface. The samples were also polished both chemically and mechanically to remove a subsurface layer several tens of micrometers thick and to achieve mirror-like surfaces.

Structural studies of the samples were conducted using electron probe microanalysis before and after cobalt diffusion. For this, the "Superprobe JXA-8800R" microanalyzer was used, which allows the study of the morphological parameters of local clusters of impurity atoms formed within the bulk of semiconductor single crystals. The sample under study is attached to a brass substrate using a conductive paint specially prepared with black carbon. The substrate is placed in a vacuum chamber with a vacuum level of 10^{-4} bar. The electron beam, generated by a tungsten filament with an accelerating voltage of 20 kV, is directed at the sample under investigation, with an excitation depth of about 20 µm. The probe current is 10 nA.

Results and discussion

Table 1 presents the results of the dependence of the sizes of the resulting micro- and nanoclusters on the cooling rate of Si<Co> n- and p-type samples after diffusion annealing. As can be seen from the table, with an increase in the cooling rate, the sizes of the impurity clusters formed within the silicon single crystals decrease. This suggests that, in the bulk of the Si<Co> samples, the majority of

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cobalt impurity atoms are attracted to smaller nanoclusters during post-diffusion quenching, resulting in an increase in their sizes.

Table 1

υ_{cool}, (K/c)		to 1	10	100	250	400
Maximum size of micro- and nanoclusters (x10^{-7} м)	n-Si<Co>	8	7	6	5	4,5
	p-Si<Co>	15	12	1	7	5

The results of structural studies of silicon samples doped with cobalt by diffusion at T=1523 K for 2 hours showed that impurity clusters formed within the bulk, with sizes reaching up to 0.5 μm and various shapes. The density of these clusters in the n-Si<Co> samples is approximately 10^3 cm^{-3}. In the surrounding crystalline structure around these clusters, dislocation lines up to several micrometers long are observed. The appearance of such dislocation lines can be explained by the fact that relatively small impurity clusters have high surface tension due to their thermodynamically nonequilibrium state [9].

The structural studies of control n-Si samples, unlike the doped samples, showed no formation of any bulk defects.

In the bulk of n-Si<Co> samples cooled at a rate of υ_{cool} = 400 K/s, impurity clusters with sizes up to 4.5×10^{-7} m were observed, mainly in the form of discs and needles. In the n-Si<Co> sample cooled at υ_{cool} = 10 K/s, impurity clusters with sizes up to 7×10^{-7} m were observed, predominantly in the form of needles and lenticular shapes. Structural studies of these samples showed that cobalt impurity clusters up to 7×10^{-7} m exert significant mechanical effects on the surrounding crystalline silicon structure. Figure 1 shows a general view of a section of the sample with impurity clusters, where dislocation lines are visible, with lengths reaching up to $\sim2\times10^{-6}$ m.

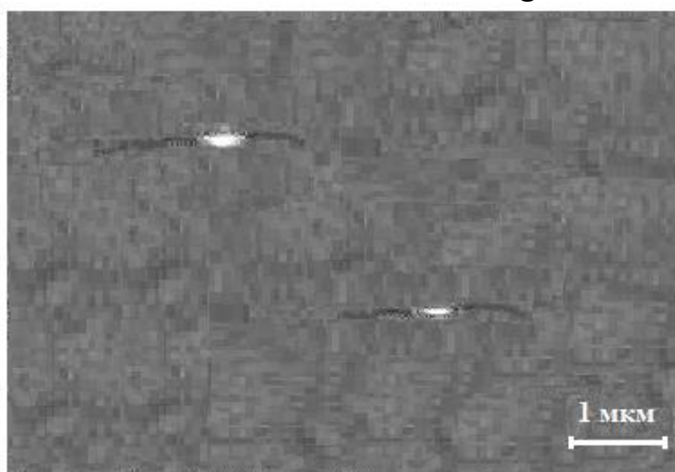

Figure. 1. Dislocation lines formed around thermodynamically nonequilibrium impurity accumulations of Co in Si.

The results of microprobe analyses of the crystalline structure around relatively large impurity clusters (≥8×10^-7 m) in p-Si<Co> samples, cooled at a rate of υcool ≤1 K/s, showed that such clusters do not exert significant mechanical effects on the surrounding crystalline silicon structure (Fig. 2). In the micrograph obtained using the

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electron probe microanalyzer, it can be seen that no dislocation lines form around the relatively large cobalt impurity clusters in silicon.

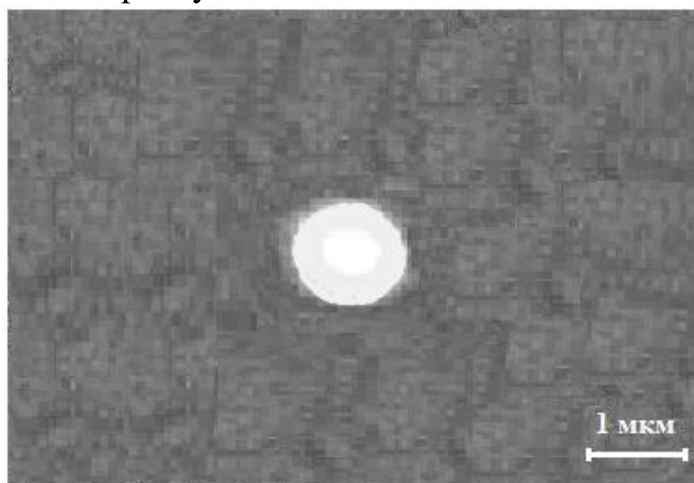

Figure. 2. General view of the surrounding structure around thermodynamically equilibrium impurity accumulations of Co in Si.

It has thus been revealed that cobalt impurity clusters with relatively small sizes ($<7\times10^{-7}$ m) significantly affect the crystalline structure of silicon, leading to the formation of dislocation lines and, in some cases, microcracks. The density and size of the dislocations formed around the microclusters depend on their size and shape, as well as their position relative to the sample surface.

Chemical composition analyses of needle-shaped and disc-shaped nanoclusters, up to 450 nm in size, in n-Si<Co> samples showed that the percentage of cobalt atoms across the entire volume of such nanoclusters is approximately 30%. This ratio of impurity atoms to the main matrix indicates that they consist of cobalt silicide, $CoSi_2$ [10]. In the near-surface regions of the nanoclusters, a sharp decrease in the percentage of cobalt atoms is observed, and in the boundary region between the impurity nanocluster and the matrix crystal, this percentage drops to about 0.5%. In other similar nanoclusters, the same percentage of impurity atoms is observed, indicating that small impurity nanoclusters consist of cobalt silicide, $CoSi_2$.

Studies of the chemical composition of relatively large nanoclusters (>500 nm) with lenticular and spherical shapes showed that they consist of two layers of silicides, $CoSi_2$ and CoSi. Depending on the shape and size of the nanoclusters, these layers can vary in thickness. The maximum percentage of cobalt atoms is found in the central part of the nanoclusters. Figure 3 shows a graph of the dependence of the percentage of cobalt atoms on the diameter of a spherical nanocluster with a diameter of d=800 nm, consisting of two layers. As seen in the graph, the percentage of cobalt atoms in the center of the nanocluster is approximately 50%, while in the surface layer, this value ranges from 30% to 33%.

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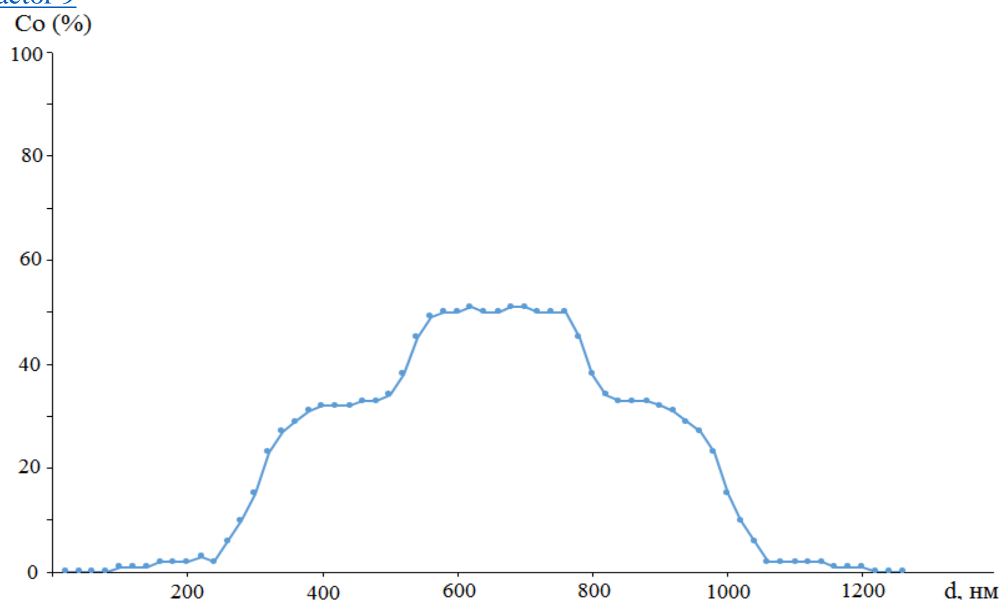

Figure. 3. Graph of the dependence of the percentage of cobalt atoms on the diameter of a spherical nanocluster with a diameter of d=800 nm

Chemical composition analyses of impurity clusters in p-Si<Co> samples, cooled slowly ($\upsilon_{cool} \leq 1$ K/s), showed that impurity nanoclusters smaller than 7×10^{-7} m also consist of cobalt silicide $CoSi_2$. Larger microclusters with lenticular and spherical shapes have a multilayer structure. These layers can vary in thickness depending on the shape and size of the microclusters. In the center of such microclusters, the percentage of cobalt atoms reaches up to ~70%.

Fig. 4 shows the graph of the dependence of the percentage of cobalt atoms on the diameter of a spherical microcluster with a diameter of $d=1.4\times10^{-6}$ m, consisting of three layers. As seen in the central part of this microcluster, the percentage of cobalt atoms reaches ~70%. In the subsequent layer, the cobalt atom content is ~48%, and in the surface layer, it is ~32%. This ratio of impurity atoms to matrix atoms indicates that these layers consist of silicides such as $CoSi_2$, CoSi, and Co_2 Si.

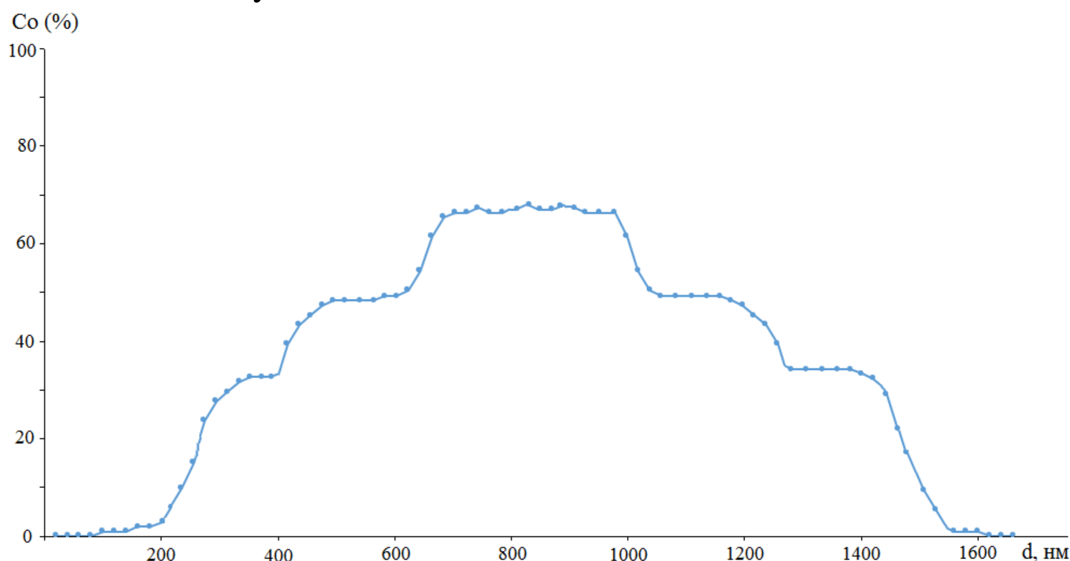

Figure. 4. Distribution of cobalt atoms across the diameter of a spherical microcluster with a diameter of $d=1.4\times10^{-6}$ m in p-Si<Co> samples.

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Based on the results of chemical composition studies of cobalt impurity clusters in silicon single crystals, it was found that the quantity and distribution of impurity atoms within microclusters depend on their size and shape. Additionally, it was established that the cooling rate of Si<Co> samples after diffusion annealing significantly affects the structural parameters and sizes of the resulting impurity microclusters.

To date, when considering the mechanisms of impurity cluster formation, little attention has been given to the role of uncontrolled impurity atoms, whose diffusion coefficients are much higher than those of the primary doping impurities. However, there is considerable experimental evidence indicating the possible involvement of technological impurity atoms in the formation of impurity clusters [11,12].

The study of the chemical composition of relatively large impurity clusters (d $\geq 7\times10^{-7}$ m) with a multilayer spherical structure showed the presence of technological impurity atoms such as Fe, Cu, and others. Comprehensive analyses of these technological impurity atoms across the volume of the microclusters revealed a distinct pattern in their distribution across the diameter of the microclusters. When analyzing each silicide layer separately, it was found that the highest concentration of technological impurity atoms is located in the center of the microclusters.

Experimental results on the distribution of iron and copper atoms within a spherical cluster with a diameter of d=800 nm showed that the percentage of Fe atoms in the central part of the cluster is ~0.4%, while in the near-surface layer, it is ~0.2%. The percentage of Cu atoms in the central part of the cluster is ~0.3%, and in the near-surface layer, it is ~0.1%. These results indicate a specific pattern in the distribution of technological impurity atoms within the volume of impurity clusters.

Conclusion

Thus, based on the results of chemical composition studies of microclusters in n-Si<Co> samples, it has been established that both monolayer and multilayer impurity clusters contain not only the primary cobalt impurity atoms but also technological impurities such as Fe, Cu, and others. A distinct pattern in the distribution of technological impurity atoms across the diameter of the clusters was observed, with the concentration of these atoms decreasing from the center toward the surface of the impurity cluster. The results of these studies indicate that the quantity and distribution of impurity atoms within cobalt clusters in silicon single crystals depend on their size and shape.

Literature:

1. Zainabidinov S.Z., Karimberdiev Kh.Kh., Shoumarova M.M., Kholbekov A.A. Structure and internal pressures in impurity nickel precipitates in silicon // UFZh. 1991. No. 4. pp. 43-46.

2. Zainabidinov S.Z., Musaev K.N., Turgunov N.A., Turaev A.R. Dopant microassociation mechanisms in Si<Mn> and Si<Ni> // Inorganic Materials. 2012. Vol. 48. Issue 11. pp. 1065-1069.
3. Fistul V.I., Turaev A.R., Zainabidinov S.Z. Baric Impurity Effects in Silicon // Phys. Stat. Soll. 1993. (a)136. P. 337-340.
4. Buonassisi T., Heuer M., Istratov A.A., Pickett M.D., Marcus M.A., Lai B., Cai Z., Heald S.M., Weber E.R. Transition metal co-precipitation mechanisms in silicon // Acta Materialia. 2007. 55. P. 6119-6126.
5. Fenninga D.P., Newmana B.K., Bertonia M.I., Hudelsona S., Bernardisa S., Marcus M.A., Fakrab S.C., Buonassisi T. Local melting in silicon driven by retrograde solubility // Acta Materialia. 2013. Volume 61. Issue 12. P. 4320-4328.
6. Bulyarsky S.V., Tsygantsov A.V. Thermodynamics of the formation of metal clusters // Journal: News of higher educational institutions. Volga region. (Penza). No. 1. 2009. pp. 139-144.
7. Yoshikawa T, Morita K, Kawanishi S, Tanaka T. Thermodynamics of impurity elements in solid silicon // Journal of Alloys and Compounds. 2010. Volume 490. Issues 1–2. P. 31-41.
8. Talanin V.I., Talanin I.E. Application of a diffusion model of the formation of growth microdefects to describe defect formation in heat-treated silicon single crystals // Physics and Technology. 2013. volume 55. issue. 2. pp. 247-251.
9. Bulyarsky S.V., Fistul V.I. Thermodynamics and kinetics of interacting defects in semiconductors. –M.: Science. 1997. 352 p.
10. Myurarka S. Silicides for VLSI. –M.:, World. 1986. -176 p.
11. Turgunov N.A. Formation of Cobalt Impurity Microinclusions in Silicon Single Crystals // Inorganic Materials, 2018, Vol. 54, No. 12. pp. 1183-1186.
12. Chang Sun, Hieu T. Nguyen, Fiacre E.Rougieux, Daniel Macdonald Precipitation of Cu and Ni in n- and p-type Czochralski-grown silicon characterized by photoluminescence imaging // Journal of Crystal Growth. 2017. Volume 460. P. 98-104