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Structures of Inclusions of Impurity Nickel Atoms in Silicon Monocrystals

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Abstract: ***Morphological parameters of microinclusions and nanoinclusions of impurity nickel atoms in silicon are studied by electron probe microscope. The dependence of the structural constructions of impurity clusters on their size and shape was studied. Quantitative indicators of the distribution of the atoms of the main and technological impurities over the volume of impurity clusters are established.***

Keywords: ***accumulations of impurity nickel atoms, morphological parameters, electron probe microanalysis.***

I. INTRODUCTION

Investigations of the processes occurring in the volume of semiconductor materials upon the introduction of impurities into them, the laws of their transformation, during which their composition and structure changes, is of particular interest from the point of view of determining the sequence of stages of formation of various accumulations of impurity atoms [1-4]. In this direction, the study of the nature of phenomena accompanying structural changes in matter, establishing the causes and methods of controlling physicochemical processes that ultimately determine the components and structural constructions of impurity clusters are most relevant. The identification of these factors is essential in the production of semiconductor materials with predetermined properties.

Currently, many leading laboratories and scientific centers of the world are conducting numerous experiments in the field of the dependence of the structure of accumulations of impurity atoms on its morphological parameters. In this regard, scanning probe microscopy is worth attention, which allows one to determine the quantitative ratios of impurity atoms and the main matrix in the volume of impurity clusters with fairly high accuracy (for metals it is 0.01%).

The results of our previous studies showed that during diffusion doping of silicon single crystals with cobalt atoms, defective structures are formed in the form of microinclusions or nanoinclusions [5-7].

It was shown that in the formation of impurity clusters, in addition to the atoms of the main impurity, atoms of uncontrolled impurities, such as copper, iron, chromium, which have relatively high diffusion and solubility coefficients, also take an active part. This paper presents the results of studies of the structural constructions and chemical composition of accumulations of nickel impurity atoms in silicon, as well as the influence of size and geometric shape on the structural constructions of microinclusions and nanoinclusions of impurity atoms.

II. MATERIALS AND METHODS

For research, we prepared samples of Si <Ni>, n- and p-type, obtained on the basis of the starting material - monocrystalline silicon of the KEF brand, with specific resistances ρ = 5 Om·cm and ρ = 20 Om·cm, respectively, grown by the Czochralski method . Nickel diffusion in silicon for both n-Si <Ni> and p-Si <Ni> samples was carried out at a temperature of 1523 K for 2 hours, after which the samples were subjected to slow and fast cooling. In the first case, the cooling rate (υ cool) of the samples was $\upsilon_{cool} \leq 1$ K / s. And with rapid cooling, it reached $\upsilon_{cool} = 100$ K / s. The method of electron probe analysis, using the Superprobe JXA-8800R setup, carried out structural studies of impurity microinclusions and nanoinclusions. In terms of its sensitivity and accuracy, this setup is superior to other analogues and allows one to determine with high accuracy the chemical composition of individual sections of impurity clusters, the sizes of which are 100-150 nm.

III. RESULTS AND DISCUSSION

The results of experimental studies have shown that the morphology of microinclusions and nanoinclusions of impurity nickel atoms formed in the silicon bulk mainly depends on the value of υ_{cool} of the samples after diffusion annealing. Figure 1 shows images of accumulations of impurity atoms in n-Si <Ni> samples obtained with a slow (a) and fast (b) cooling rate. As can be seen in the volume of n-Si <Ni> samples obtained with slow cooling, impurity clusters with sizes ranging from several hundred nanometers to ~ 5×10^{-6} m are formed. The resulting clusters of impurity atoms, with relatively small sizes up to ~ 800 nm, i.e. impurity nanoinclusions have a needle-shaped, disk-shaped, lenticular and spherical shape. In contrast, larger impurity clusters, the sizes of which reach up to several micrometers, i.e. impurity microinclusions have mainly a convex lenticular or spherical shape,

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as well as a complex multifaceted shape with a multilayer structure, the boundaries of which are clearly distinguished (Fig. 1 (a)). Depending on the shape and the size of multilayer microinclusions, each layer may have different thicknesses.

The density of such microinclusions according to the volume of the samples is on average ~ 10^2 cm^{-3}.

In the volume of n-Si <Ni> samples obtained with υ_{cool} = 100 K / s, the formation of mainly referring to small clusters of impurity atoms is observed, the sizes of which reach up to 700-800 nanometers, and their average density is ~ $2{\cdot}10^3$ cm^{-3}. Such nanoinclusions have needle-shaped, disk-shaped, lenticular, and spherical shapes (Fig. 1 (b)). Lenticular clusters, in turn, can have biconvex, plano-convex, plano-concave or convex-concave forms (Fig. 1 (b)).

The results of the analysis of the chemical composition of the impurity microinclusion with a spherical shape, diameter d = $1.9{\cdot}10^{-6}$ m, which has a three-layer structure are shown in Fig. 2. As can be seen, nickel atoms are distributed unevenly over the diameter of the impurity microinclusion. In the central layer of microinclusion, the percentage of nickel atoms reaches 50%, and toward the surface this value decreases by a spasmodic character. In the subsequent microinclusion layer, this value substantially decreases and amounts to ~ 32%. And on the surface layer, it decreases even more and equals to ~ 25%. As it turned out, a certain regularity is observed in the distribution of nickel atoms along the diameter of multilayer microinclusions (d≥10^{-6} m), according to which the percentage of impurity atoms increases towards the center of microinclusions and in this region it reaches its maximum value.

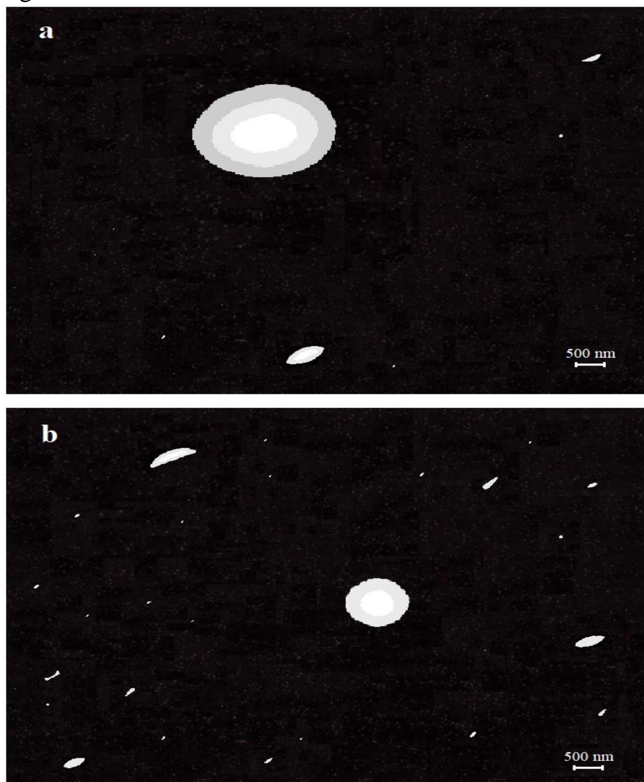

Fig. 1. Pictures of accumulations of nickel impurity atoms in n-Si <Ni> samples obtained with a slow (a) and fast (b) cooling rate.

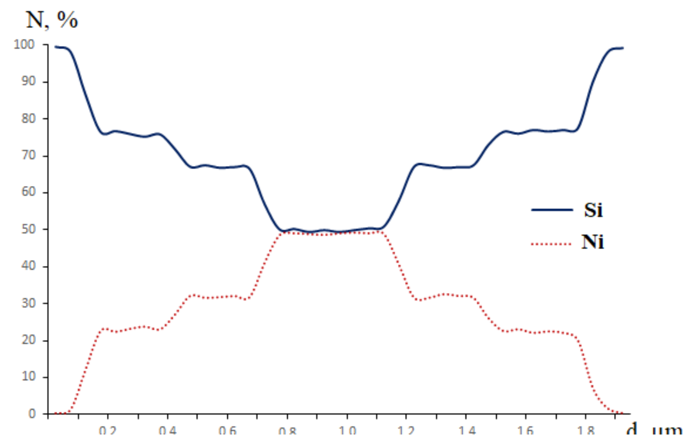

Fig. 2. The distribution of Si and Ni atoms over the diameter of the microinclusion, having a three-layer structure with a spherical shape, with a diameter d = $1.9{\cdot}10^{-6}$ m.

The obtained micrographs of n-Si <Ni> samples with rapid cooling showed that relatively small clusters of impurity atoms (d≤500 nm have a single-layer structure. The results of a quantitative analysis of nanoinclusions of a convex lenticular shape with a diameter of 600 nm are shown in Fig. 3. Graph of the distribution of nickel atoms the volume of this nanoinclusion shows that it has the same value over the entire diameter and amounts to ~ 25%. Analysis of the chemical composition of such impurity nanoinclusions confirms that nickel atoms are distributed in their volumes uniformly, i.e. they have a homogeneous structure (Fig. 3).

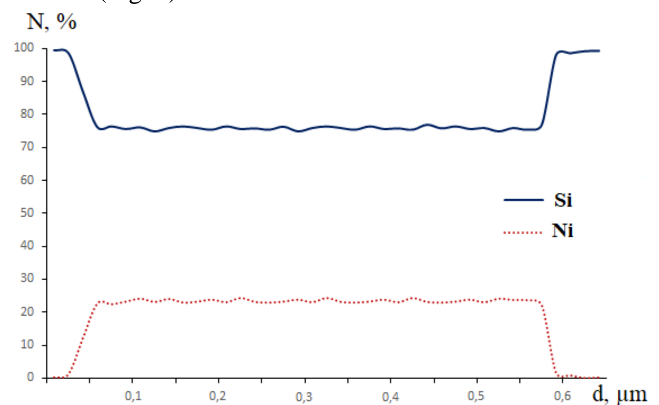

Fig. 3. Distribution of Si and Ni atoms over the diameter of the nanoinclusions, d = 600 nm in size with a lenticular shape.

As is known, at high temperatures of diffusion annealing, the atoms of technological impurities have a significant effect on the formation of microinclusions [8, 9]. Currently, when studying the mechanisms of formation of clusters of impurity atoms in the volume of semiconductor silicon, special attention is paid to the role of atoms of technological impurities in the process of their formation. Since the diffusion coefficient of atoms of technological impurities is much higher in comparison with the atoms of the main dopant, there are some assumptions that indicate the

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possible active participation of atoms of technological impurities in the formation of the structure of impurity clusters [10, 11].

The results of analyzes of the chemical composition of impurity microinclusions and nanoinclusions in n-Si <Ni> samples obtained both with fast and slow cooling showed that atoms of technological impurities such as Fe and Cr exist in their volume. The analyzes performed for a spherical microinclusion with a diameter of $d = 1.9 \cdot 10^{-6}$ m, having a three-layer structure, made it possible to determine the quantitative indicators of atoms of technological impurities of iron and chromium in each shell of the microinclusion. The dependence of the percentage of atoms of uncontrolled impurities on the diameter of the microinclusion is shown in Fig. 4. As can be seen, the percentage of iron atoms in the central part of the microinclusion is ~ 0.16%, and for Cr atoms it is ~ 0.12%. In the subsequent layer of microinclusion, the percentage of Fe and Cr atoms decreases to ~0.1% and ~0.8%, respectively. And in the surface layer, these values decrease to ~ 0.07% and ~ 0.04%, respectively.

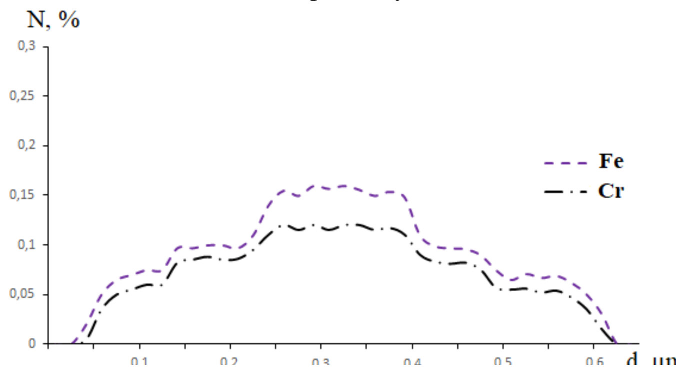

Fig. 4. The distribution of atoms of technological impurities Fe and Cr along the diameter of the microinclusion, having a three-layer structure with a spherical shape, with a diameter of $d = 1.9 \cdot 10^{-6}$ m.

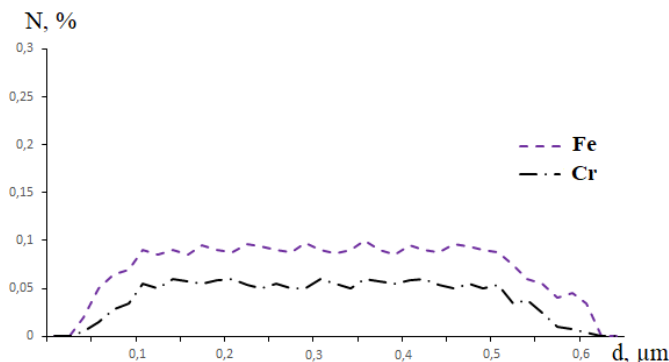

Fig. 5. The distribution of atoms of technological impurities Fe and Cr by the diameter of the nanoinclusions, d = 600 nm in size with a lenticular shape.

In the course of studying the distribution of atoms of technological impurities over the volume of multilayer impurity clusters, it turned out that there is a certain regularity in their distribution over the diameter of microinclusions. In accordance with this pattern, the maximum percentage of atoms of technological impurities are located in their central part. In the direction from the center to the surface of impurity clusters, the percentage of atoms of these impurities decreases.

IV. CONCLUSION

Thus, on the basis of the results obtained, it was revealed that with an increase in the υ_{cool} value, the probability of the formation of impurity nanoinclusions with relatively small sizes that have a needle-shaped, disk-like, lamellar and lenticular shape increases. At low values of $\upsilon_{cool} \leq 1$ K / s, larger nanoinclusions are formed, which consist of several layers and have mainly a lenticular and spherical shape. It has been established that the number and distribution of impurity atoms over the volume of nanoinclusions depend on their size and shape. Morphological parameters of impurity nanoinclusions, i.e. the structural constructions, chemical composition, geometric shapes and sizes mainly depend on the cooling rate of the samples after diffusion annealing. In samples with a high cooling rate, after diffusion annealing, impurity nanoinclusions of various shapes are formed with relatively small sizes (up to 500 nm) and they have a single-layer structure. At low cooling rates, lenticular and spherical nanoinclusions are formed with sizes up to ~900 nm, which have a multilayer structure. It was established that in the volume of impurity nanoinclusions there are atoms of technological impurities like Fe and Cr. It turned out that a certain regularity is observed in the distribution of atoms of technological impurities over the diameter of nanoinclusions, according to which the percentage of atoms of these impurities decreases in the direction from the center to the surface of the nanoinclusions.

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