FORMATION AND MORPHOLOGY OF PHOSPHORUS AND NICKEL IMPURITY ATOM CLUSTERS IN SILICON DURING SEQUENTIAL DOPING AND THERMAL ANNEALING

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Abstract
This study investigates the effect of sequential doping of silicon with phosphorus and nickel on the formation, size, and morphology of impurity clusters. P-type silicon wafers obtained by the Czochralski method were subjected to phosphorus diffusion to form a p-n junction, followed by nickel deposition and high-temperature diffusion, with a final thermal annealing process. The resulting cluster structures were analyzed using scanning electron microscopy (SEM). The formation of precipitates of various shapes and sizes was observed, including oval and round clusters ranging from nanometers to several micrometers. A correlation between technological process parameters and the characteristics of the formed clusters was established. The results enhance the understanding of impurity atom interactions in silicon and open prospects for developing new methods for controlled impurity structure formation.
Keywords: cluster formation, phosphorus, nickel, silicon, thermal annealing, scanning electron microscopy.

Introduction

Doping silicon with various impurities is a fundamental process in the technology of semiconductor device fabrication, determining their electrophysical properties. Of particular scientific and practical interest is the study of the effects of co-doping with donor and metallic impurities on the microstructure of silicon, as well as the influence of subsequent thermal treatments on the redistribution and clustering of impurity atoms.

Literature Review

It is well known that doping with phosphorus leads to saturation of carrier concentration, which is associated with the formation of clusters containing several impurity atoms. In [1], a model was proposed for the formation of negatively charged phosphorus clusters in silicon, consisting of two to four atoms, which explains the limitation in conductivity levels at high doping concentrations.

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The formation of nickel clusters is also a complex process that depends on temperature regimes and the conditions under which the impurity is introduced. In [2], it was shown that sequential doping and controlled annealing make it possible to manipulate the morphology of nickel clusters, including their size and density. Using infrared microscopy, it was established that nickel clusters can be evenly distributed within the silicon crystal and form stable structures, especially under additional irradiation [3].

When nickel is implanted into silicon, as demonstrated in [4], epitaxial silicides are formed on the surface, which can be utilized in the technology for creating conductive layers. Furthermore, in [5], it was demonstrated that introducing nickel atoms followed by thermal treatment significantly broadens the spectral sensitivity of silicon solar cells due to the emergence of intermediate energy levels.

Nickel doping and subsequent annealing of silicon can lead to improved solar cell parameters, including increased carrier lifetime and reduced recombination losses [6]. A comprehensive analysis of deep levels in doped silicon, conducted in [7], identified defects associated with nickel-hydrogen complexes, which is important for understanding degradation processes in such devices.

Special attention should be given to theoretical studies such as [8], where, using density functional theory methods, it was shown that phosphorus tends to segregate within the crystal volume, unlike boron, which can significantly affect impurity behavior during annealing.

This study is aimed at investigating the influence of sequential doping of silicon with phosphorus and nickel on the formation, size, and morphology of impurity clusters under additional thermal treatment.

Methods

Materials and Sample Preparation

The initial materials used were monocrystalline p-type silicon wafers grown by the Czochralski method, boron-doped, with a specific resistivity of 0.5 Ω·cm and a thickness of 380 μm.

The sample preparation process included the following stages:

1. Formation of a p-n junction by gas-phase diffusion of phosphorus at 1000°C for 30 minutes.
2. Vacuum deposition of a 1 μm thick layer of pure metallic nickel onto the surface of the samples with a p-n junction.
3. Nickel diffusion at 1200°C for 30 minutes.
4. Additional thermal annealing at 1000°C for 30 minutes.

Research Methods

To examine the size and morphology of the resulting impurity atom clusters, scanning electron microscopy (SEM) was used. The analysis was carried out at two magnification levels: x1,500 (field of view 85.33 × 64.00 μm) and x10,000 (field of view 12.80 × 9.60 μm). The investigations were performed in secondary electron detection (SED) mode at an accelerating voltage of 15.0 kV and a working distance of 11.7 mm.

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Results

Analysis of SEM images of silicon samples sequentially doped with phosphorus and nickel followed by thermal annealing revealed the formation of various cluster structures. In the SEM image at x1,500 magnification (Figure 1, left panel), a non-uniform distribution of impurity atom clusters across the sample surface is observed. The clusters predominantly exhibit a round shape with size variations ranging from 0.5 to 5 µm. Green markers on the image indicate the measurements of individual cluster sizes, demonstrating their diverse diameters.

At higher magnification (x10,000, Figure 1, right panel), a more detailed morphology of the clusters is revealed. It can be seen that large clusters (>1 µm) exhibit a well-defined rounded shape with relatively smooth boundaries, whereas smaller clusters display more complex morphologies, often with irregular oval shapes and uneven edges. The largest visible cluster (marked with a green indicator) has a diameter of approximately 3 µm and a regular circular shape.

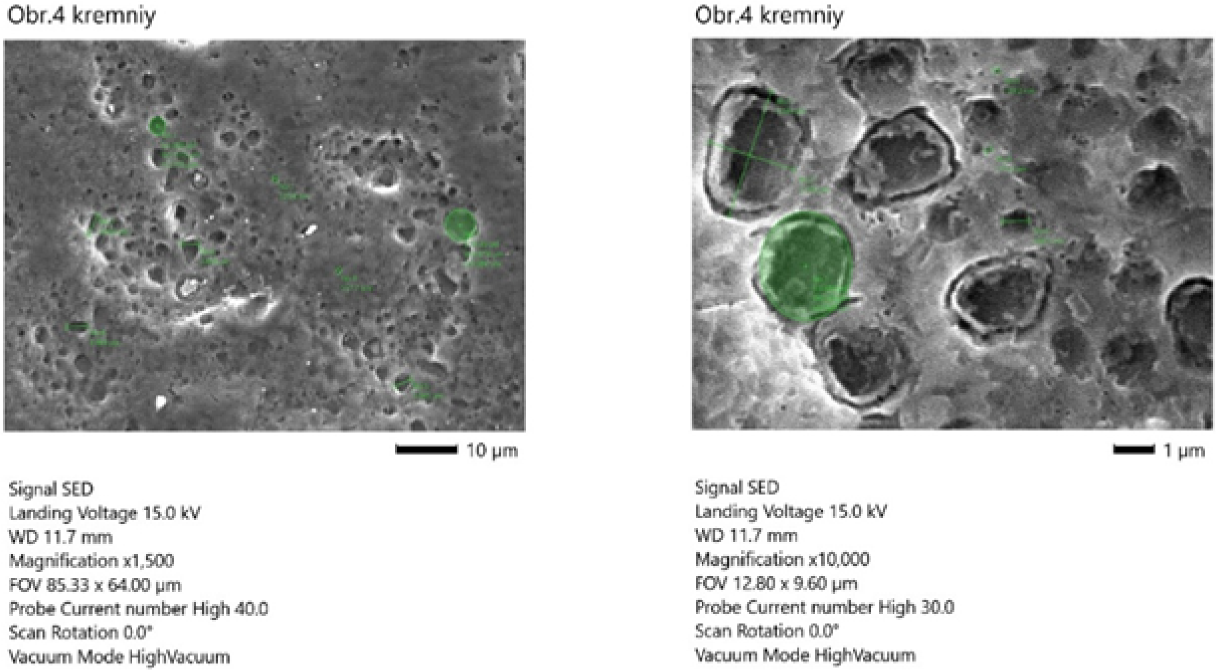

Figure 1. *SEM images of silicon samples sequentially doped with phosphorus and nickel after thermal annealing. Left: general view of the distribution of impurity clusters at ×1,500 magnification (scale bar 10 µm). Right: detailed image of the morphology of individual clusters at ×10,000 magnification (scale bar 1 µm). Green markers indicate measurements of representative cluster sizes. The images were obtained in secondary electron detection (SED) mode at an accelerating voltage of 15.0 kV. A characteristic feature of the observed clusters is the presence of a structured internal region, which may indicate a complex composition and the possible formation of nickel silicides or complexes involving phosphorus atoms. Additionally, areas with altered surface morphology around some large clusters suggest the redistribution of defects and impurity atoms during thermal processing.*

Discussion

The results obtained from SEM analysis allow conclusions to be drawn regarding the mechanisms of impurity cluster formation in silicon during sequential doping with phosphorus and nickel.

The observed variety in cluster sizes (from nanometers to several micrometers) indicates the complex kinetics of impurity atom diffusion and precipitation processes. It can be assumed that initial phosphorus doping and the formation of the p-n junction create a nonuniform distribution of defects and electric fields within the silicon structure, subsequently affecting the diffusion and precipitation of nickel atoms.

The characteristic morphology of large clusters with relatively regular round shapes suggests that thermodynamic equilibrium was achieved during their formation. In contrast, the irregular shape of smaller clusters may indicate a nonequilibrium state or the influence of the local defect and impurity environment.

The internal structure of the observed clusters suggests that they may not be simple nickel precipitates, but rather complex formations involving phosphorus atoms. The additional thermal annealing at 1000°C likely facilitated the redistribution of impurity atoms and the formation of more stable cluster structures.

Changes in surface morphology around large clusters may point to the generation of additional defects during the precipitation process.

The results demonstrate the feasibility of controlled formation of impurity clusters with specific sizes and morphologies by adjusting doping and thermal treatment parameters, which may have practical significance for modifying the electrophysical properties of semiconductor structures.

Conclusion

In this study, scanning electron microscopy was used to investigate the formation of impurity atom clusters in silicon during sequential doping with phosphorus and nickel followed by thermal annealing. It was found that the applied technological sequence leads to the formation of impurity clusters of various shapes and sizes, ranging from nanometers to several micrometers.

The morphology and distribution of the clusters are linked to the parameters of the doping and thermal processing steps. The observed structural features of the clusters indicate a complex nature of the interaction between phosphorus and nickel impurity atoms and the defects in the silicon crystal lattice.

The findings expand the understanding of impurity cluster formation mechanisms in silicon and can be applied in developing new methods for controlled modification of semiconductor material properties for microelectronics.

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