

INVESTIGATION OF DIFFUSION-DOPED SILICON WITH ZINC AND SELENIUM ATOMS

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Abstract. The currently existing technological methods for obtaining semiconductor materials for the development of efficient photocells with maximum efficiency and stable electrical parameters have almost reached their limit. To further increase the main parameters of photocells, it is necessary to use non-traditional properties of semiconductor materials or requires discovered new physical phenomena. The modern development of micro- and optoelectronics arouses interest in the synthesis of new materials, including those based on A^3B^5 and A^2B^6 semiconductor compounds. Since the band gap and lattice constant of such compounds vary within certain limits, depending on the concentration of impurity atoms, which affects the fundamental parameters of such materials. Based on them, it is possible to synthesize semiconductor materials with a wide range of electrical and photoelectric properties, as well as superlattices with quantum dots.

Keywords: diffusion, X-ray phase analysis, silicon, selenium, zinc, relief, compounds, nanocrystal, reflex, cluster, structure.

Introduction

The development of modern micro- and nanoelectronics requires the creation of new materials and devices based on them, with energysaving properties and new functional capabilities. In this regard, nanostructured silicon doped with impurity atoms is of great interest. These materials can be obtained by forming clusters of various impurity atoms; however, as studies have shown, the resulting materials do not fully address the challenges of modern nanoelectronics [1]. This is primarily due to the low concentration, as well as the inability to control the concentration and composition of the impurity nanoclusters in silicon. Therefore, a new type of nanostructured binary clusters involving elements from groups II and VI in silicon lattices is of significant interest. According to literature data, these impurity atoms in silicon exhibit high solubility ($N = 1020\text{--}1021\text{ cm}^{-3}$). In isolation, these atoms create small donor and acceptor levels, which in turn introduce additional electrons into the conduction band and holes into the valence band.

The aim of this research is to study the surface states using X-ray phase analysis of the diffusion layer $(\text{Si}_2)_{1-x}(\text{ZnSe})_x$ formed on a silicon substrate. The structures were obtained by the diffusion method from a confined volume, using the technology described in [2].

The diffusion layer $(\text{Si}_2)_{1-x}(\text{ZnSe})_x$ was obtained based on the initial silicon of grade KEF-100, with a crystallographic orientation of $\langle 111 \rangle$ and a diameter of 20 mm. The resulting silicon-based films were of n-type conductivity with a thickness of approximately 5 μm . To determine the elemental composition of the silicon surface, samples were analyzed using an X-ray microanalyzer of the "Jeol" JSM 5910 LV-Japan brand. The results of these studies showed that the distribution of components in the volume of the diffusion layer $(\text{Si}_2)_{1-x}(\text{ZnSe})_x$ changes to a depth of $x = 5\text{ }\mu\text{m}$. Figure 1 shows the profile of the component distribution by depth in the diffusion layer. As seen from the figures, in the diffusion layer of the type $(\text{Si}_2)_{1-x}(\text{ZnSe})_x$, the content of the molecular compound ZnSe increases non-monotonically, which can be explained by the undersaturation relative to the ZnSe molecules. Further, the content of ZnSe quickly increases, reaching a maximum value at $x = 5\text{ }\mu\text{m}$ from the surface. Since the layer growth

occurs in a confined volume, as the diffusion layer grows, the concentration of ZnSe molecules decreases, which leads to a gradual reduction in the molar fraction of ZnSe in the newly formed solid phase [3-4].

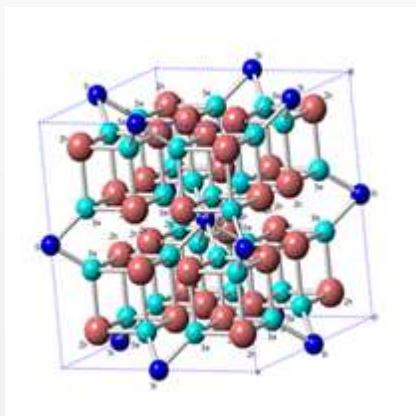


Fig. 1. Formation of binary elementary cells of the type $(\text{Si}_2)_{1-x}(\text{ZnSe})_x$ in silicon with ionic-covalent bonding.

Experimental Methodology

This work examines the physical principles of the formation of electron-neutral molecules between atoms of group II and VI elements, located at neighboring nodes of the silicon lattice (Fig. 1).

As seen from the proposed model, the atoms formed in the new clusters are neither purely covalent nor purely ionic in nature but form a strong ionic-covalent bond. According to the proposed model, clusters of the type $(\text{Si}_2)_{1-x}(\text{ZnSe})_x$ act as a separate material in the crystalline lattice of silicon, forming compounds and associations of binary structures A_2B_6 individually. The formation of such compounds leads to changes in the electrical and optical properties, which can be considered as a fundamentally new material for silicon-based electronics [5].

On the surface and within the volume of the new material, the formation of ionic bonds of the ZnSe type leads to the appearance of nanoclusters, within which p-n junctions are formed, as well as changes in the mobility and lifetime of charge carriers and the light absorption coefficient. The formation of these electron-neutral molecules does not disrupt the tetrahedral chemical bond of the silicon lattice. Moreover, these impurities do not create additional electrons in the conduction band or holes in the valence band, which also affects the electrophysical parameters of silicon [6]. When these impurity atoms are present in the lattice in an isolated atomic state, due to ionization, they create an electric potential around them, which is also a defect in the lattice.

When electron-neutral molecules form between atoms of group II and VI, no additional energy levels are created in the forbidden band of silicon, i.e., no additional charge carriers appear. Particularly, the formation of molecules takes into account the high concentration of impurity atoms. In the state of molecular compounds, the atomic potential is shielded between them, with Coulomb interactions also to be considered [7]. These mechanisms of ionic bond formation are a stimulating factor for the formation of electron-neutral molecules and ensure the most thermodynamically stable state. Therefore, it can be assumed that under certain conditions, elements of groups II and VI will participate in the formation of molecular compounds.

When electron-neutral molecules are formed, new elementary cells of the type $(\text{Si}_2)_{1-x}(\text{ZnSe})_x$ are created. The concentration and distribution of these binary elementary cells are mainly determined by diffusion, i.e., by the temperature and diffusion time of the impurity atoms of zinc and selenium in silicon [8].

(220) reflection, the lattice parameter of the binary ZnSe compound was determined, which was found to be $\text{ZnSe} = 5.692 \text{ \AA}$, slightly larger than the fundamental lattice parameter of pure binary ZnSe ($5.661 \text{ \AA}$). Therefore, the obtained layer has the following composition: $(\text{Si})_{1-x}(\text{ZnSe})_x$.

Discussion of Results

New binary compounds with ionic bonds of the ZnSe type form on the surface and within the volume of silicon. This leads to the appearance of nanoclusters within the silicon volume, which conduct and form p-n junctions. In such silicon materials, the formation of binary compounds leads to changes in the mobility and lifetime of charge carriers, as well as in the light absorption coefficient. It was established that the formation of these electron-neutral molecules does not disrupt the tetrahedral chemical bond of the silicon lattice. Moreover, molecular compounds of the ZnSe type do not create additional electrons in the conduction band or holes in the valence band, which also causes further changes in the electrophysical parameters of silicon [10].

Conclusion

The developed technology for doping by the diffusion method with impurity atoms of zinc and selenium demonstrated the possibility of creating and controlling the concentration of binary ZnSe compounds, which allows the management of the fundamental photoelectric and optical properties of the obtained materials. The analysis of the presented research shows that the binary compounds of the type $(\text{Si})_{1-x}(\text{ZnSe})_x$, formed in silicon, enable the development and creation of semiconductor lasers and efficient solar cells of a new generation. As known from the literature, monocrystalline silicon, although it is the primary material in the electronics industry, cannot be used to create emitting devices and lasers for optoelectronics.

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