Section 6. Physics

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FUNDAMENTAL MANAGEMENT (E_g, μ BAND STRUCTURE) SILICON IS A NEW DIRECTION IN THE FIELD OF SEMICONDUCTOR MATERIALS

Abstract. In this paper, we consider the physical foundations for the formation of electronetral molecules between atoms of groups *III* and *V*, as well as elements of groups *II* and *VI* located in neighboring sites of the silicon lattice. Elements will participate in the formation of molecules. Preliminary results have shown that in the case of formed elementary cells $Si_2Zn - Se^{++}$ with a maximum concentration, E_g – varies from 1.35 to 1.12 eV and, accordingly, from 2.67 to 1.12 eV.

Keywords: silicon, Kloun interactions, nanoclusters, heterovarigone structures, selenium, zinc.

1. introduction

The development of modern micro and nanoelectronics requires the creation of new materials with unique energy properties and functionality. In this regard, nanostructured semiconductors based on silicon are of great interest. Although such materials can be obtained by the formation of clusters of various impurity atoms [1–2], studies have shown that the preparation of such materials does not allow solving problems in modern nanoelectronics. This is mainly due to the low concentration, distribution control and composition of impurity nanoclusters in silicon. Therefore, the formation of a new type of binary cluster nanostructures with the participation of elements of groups *III* and *V*, as well as *II* and *VI* groups in silicon lattices is of great interest. The valences of groups *III* and *V* in silicon have a high solubility (N – 10^{20}–10^{21} cm). In a separate state, they create shallow donor and acceptor levels, and they, in turn, create additional electrons in the conduction band and holes in the valence band.

This paper discusses the physical foundations for the formation of electronetral molecules between atoms of *III* and *V* groups, as well as *II* and *VI* groups of elements located in neighboring sites of the silicon lattice (Fig. 1.).

As can be seen from the model, the new material is neither covalent nor ionic and formed a bond, but a strong bond with an ionic-covalent appearance was obtained. According to the proposed model, the crystal type $Si_2A^{II}B^{VI}$ as a separate material in the lattice of compounds itself and the association of $A^{II}B^{VI}$ structures separately, the compound is displayed. This is a brand new material.

Being, it does not repeat its basic properties and processes in it will not be the same as in the first example. Including the surface of the new material, and due to $Zn^{++}Se^{-}$ nanoclusters in local places of the volume, transitions and mobility occur, the life of charge carriers and absorption coefficients will also be different. During the formation of such electrically neutral molecules, the tetrahedral chemical

bond of the silicon lattice is not disturbed. At the same time, these impurities do not create additional electrons in the conduction band and holes in the valence band, which are also lattice defects.

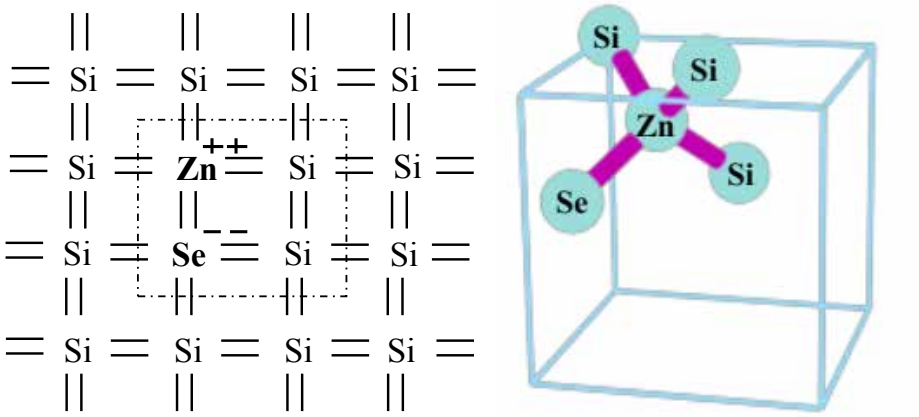

Figure 1. Formation of binary elementary cells Si_2Zn-Se^{++} in silicon with ionic-covalent bonds

When these impurity atoms are in a lattice without formed molecules, each of them creates an electric potential around itself, which is also a lattice defect. During the formation of electrically neutral molecules between the atoms of groups *III* and *V*, as well as groups *II* and *VI*, no energy levels are created in the band gap of silicon, i.e. no additional charge carriers appear. Especially in the formation of molecules, the presence of a high concentration of impurity atoms is taken into account. In the state of a molecule, the energy potential of each atom is shielded from each other, while it is necessary to take into account the Coulomb interactions. All of the above is a stimulating factor in the formation of electrically neutral molecules and provides the most thermodynamic equilibrium state. Therefore, it can be assumed that, under subtle practical conditions, elements of groups *III* and *V*, as well as *II* and *VI* groups, will participate in the formation of molecules. When electrically neutral molecules are formed, new elementary cells of the Si_2Zn-Se^{++} type are formed. The concentration and distribution of such binary elementary cells is mainly determined by diffusion, i.e. temperature and diffusion time.

2. Methodology

As shown by the preliminary results of the experiment, it is possible to form such unit cells up to a concentration of $N - 10^{20} - 10^{21} cm^{-3}$ (Fig. 2.), and their distribution over the depth of the sample is described:

$$N = (N_1 \cdot N_2)^{-1/2} \cdot erfc\left(-\frac{x}{\sqrt{2\left(\frac{D_1 + D_2}{2}\right)t}}\right)$$

where D_1 and D_2 are the diffusion coefficient, N_1 and N_2 are the solubility of impurity atoms in silicon at the diffusion temperature, and t is the diffusion time.

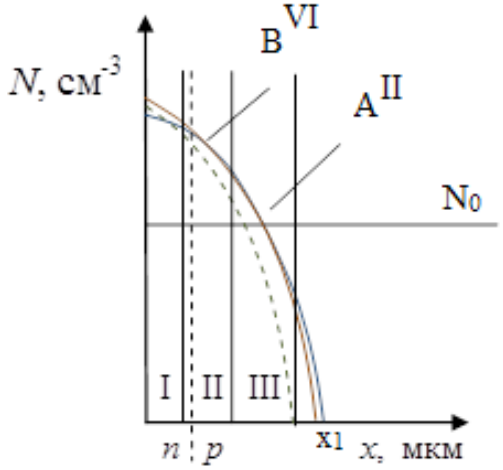

Figure 2. Concentration distribution of clusters based on $A^{II}B^{VI}$ binary nanocrystals

3. Result and discussion

Calculations and excrement show that the x_1 – value can be controlled from 0.5 to 10 μm. The results of studying the elemental composition of structures obtained based on binary compounds of the

Si_2Zn-Se^{++} type, binary compounds Si_2Zn-Se^{++} are indeed formed on the surface on the analyzer <<Jeol>> JSM 5910 LV-Japan (Fig. 3).

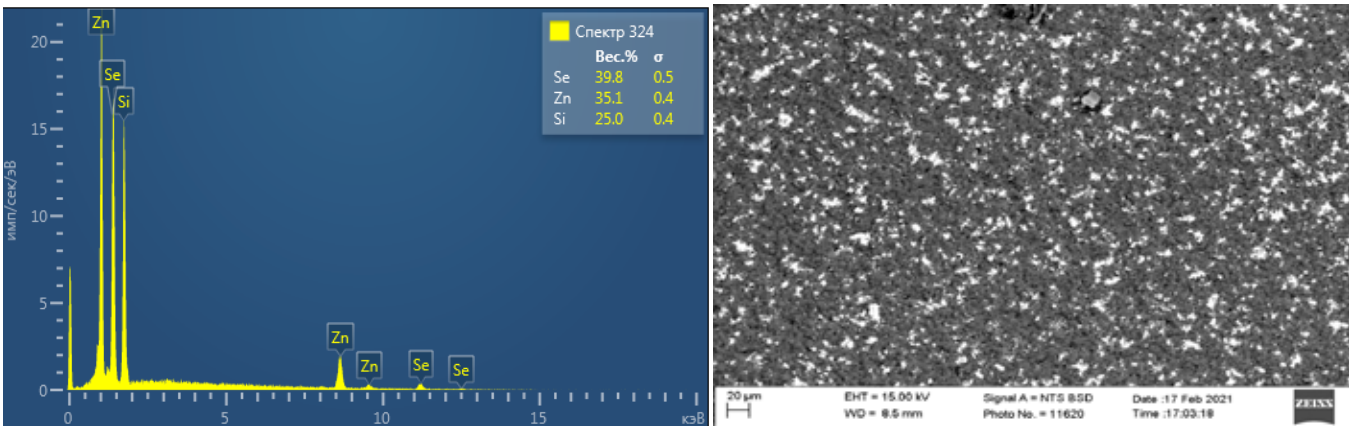

Figure 3. Results of *X*-ray microanalysis of the Si_2Zn-Se^{++} structure after diffusion at T = 1200 °C, t = 2 *h* on the silicon surface

In this surface layer, the electrical properties (carrier concentration, mobility, and band gap) were almost the same as those of pure *ZnSe* binary compounds. As the depth increases, the concentration of binary compounds decreases and the complex passes to the next neutral compound of the Si_2Zn-Se^{++} type. The results of studying the absorption spectra on the SHIMADZU UV 1900 i setup showed a decrease in the concentration of zinc and selenium impurity atoms relative to the surface (Fig. 4).

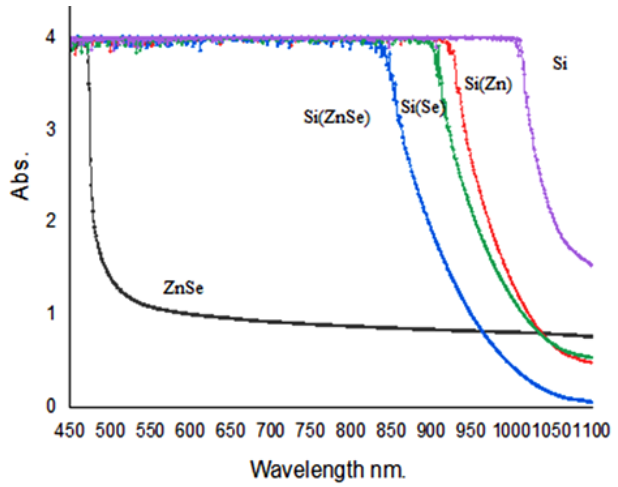

Figure 3. Absorption spectra versus wavelength of *ZnSe* and $Si_2(ZnSe)$, *Si(Se)*, *Si(Zn)* crystals measured at 300 K after diffusion at T = 1200 °C, t = 2 *h* on the silicon surface

The analysis of the obtained research results corresponded to the results of theoretical calculations, which made it possible to obtain heterovarigone structures in a silicon matrix with control over the concentration of zinc and selenium impurity atoms. We have shown the production of graded-gap structures due to the formation of binary neutral compounds of the *ZnSe* type. In the silicon lattice, which makes it possible to control the band gap of such structures with the help of additional thermal annealing. The physical parameters of new binary elementary cells are determined by the basic physical properties of materials where the concentration of binary elementary cells is high.

4. Conclusion

And the parameters of these cells E_g, μ band structure will differ significantly from the lattice parameters, as well as from the parameters of the *ZnSe* crystal. Thus, at the surface of a silicon crystal, an almost new semiconductor material is created, with new fundamental parameters. These new fundamental parameters mainly depend on the concentration of binary elementary cells. Preliminary results showed that in the case of the formation of Si_2Zn-Se^{++} unit cells, the maximum E_g concentration varies from 1.35 to 1.12 eV and, accordingly, from 2.67 to 1.12 eV, i.e. in the x_1 region, a graded-gap

heterostructure is obtained. In this region, the value of the band gap varies smoothly, and the electron mobility and band structure should also change. Currently, such studies are being carried out both in experimental and theoretical aspects. And they are also conducted on the basis of modern microscopic and *X* – ray diffraction analyzes in order to clearly determine the distribution of binary elementary cells along the depth of the sample. It should also be noted that the diffusion technology of formation proposed by us is a unique technological solution that allows you to control the fundamental parameters of the main electronics material – silicon.

Now a few words about the unique functionality of silicon enriched with binary elementary cells. Based on such materials, it is possible to create photocells with a maximum absorption coefficient in a wide spectral region, with the help of which we can create highly efficient photocells with an efficiency no worse than that of multistage photocells based on *III–V*. This allows to significantly reducing the cost of photovoltaics, which is used on a large scale in earth conditions. In addition, based on such materials it is possible to create a highly sensitive photodetector operating in a wide range of the spectrum. In the future, with the improvement of technologies, it will be possible to obtain such materials based on silicon, with the help of which it is possible to create a highly efficient emitting device with various wavelengths. Further study of physical, optical, photoelectric properties allows us to discover a number of unknown new physical phenomena with unique functionality.

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