Journal of Nano- and Electronic Physics
Vol. **15** No 6, 06024(4pp) (2023)

Журнал нано- та електронної фізики
Том **15** № 6, 06024(4cc) (2023)

New Technological Solution for the Tailoring of Multilayer Silicon-based Systems with Binary Nanoclusters Involving Elements of Groups III and V

N.F. Zikrillayev[1], S.B. Isamov[1], B.O. Isakov[1], T. Wumaier[2], Li wen Liang[2], J.X. Zhan[2], T. Xiayimulati[2]

[1] *Tashkent State Technical University, 100095, Tashkent, Uzbekistan*
[2] *Xinjiang Institute of Engineering, 830023, Urumchi, China*

(Received 26 August 2023; revised manuscript received 14 December 2023; published online 27 December 2023)

The diffusion technology has been developed for the formation of binary clusters involving elements of group III and V in silicon. It is shown that by controlling the concentration of elements of group III and V atoms, multilayer silicon-based heterojuns can be formed in the surface region of silicon with enriched AIIIBV nanocrystals, followed by enriched with various combinations of Si2AIIIBV unit cells (1 – 5 μm thick). This creates a practical new material based on silicon - a continuous graded-gap structure, i.e. heterojuns by a smooth transition from the band gap of III – V semiconductor compounds to the band gap of silicon.

Keywords: Semiconductor, Binary clusters, Muticascade PV Cells, Elementary Cells, Self-Organization, Self-Structure, Nanostructure, Nanocrystal, Photosensivity, Combinations, Multistage PV cells.

DOI: 10.21272/jnep.15(6).06024 PACS numbers: 61.72.uf, 68.43.Jk

1. INTRODUCTION

In modern electronics and photovoltaics, silicon still remains as the main material. Further use of silicon is significantly limited due to its functionality. For example, the value of the silicon band gap limits the absorption both in the UV and in the visible region of the solar energy spectrum. The relatively small value of electron mobility limits the use of this material in the development and creation of high-speed electronic devices. Also indirect band gap structure of silicon does not allow creating lasers based on it [1].

In this work, a new technological approach is proposed for forming heterostructures in a silicon lattice. The heterojunction structure is formed on the basis of binary unit cells of III-V semiconductor compounds in the silicon lattice with specified parameters [2-5].

2. THEORETICAL ANALYSIS

The results of our studies over the past 15 years show that there are optimal conditions for doping of silicon with impurity atoms of groups III and V, which allow impurity atoms to be inserted adjacent to neighboring sites in the silicon crystal lattice (Fig. 1), where they form the electroneutral molecule $A^{III}B^{V}$. In this case, a completely newhidden heterostructure with unit cells of the $Si_2A^{III}B^{V}$ type in the silicon lattice (dashed lines indicate the conditional boundary of the heterostructures).

This is due to the fact that, firstly, during the formation of electroneutral molecules $A^{III}B^{V}$, the electric potentials of ions A^{III} and B^{V} almost completely shield each other, while these atoms do not create any additional energy levels in the band gap of silicon, i.e. "impurity" electrons do not appear in the conduction band or holes in the valence band. This means that the level of defectiveness of the system is significantly reduced. Secondly, the formation of new binary unit cells of $Si_2A^{III}B^{V}$ practically does not violate the tetrahedral covalent bond in the silicon lattice. Therefore, the formation of electrically neutral molecules between atoms of groups III and V stimulates the self-organization and independent formation of binary unit cells in the silicon lattice.

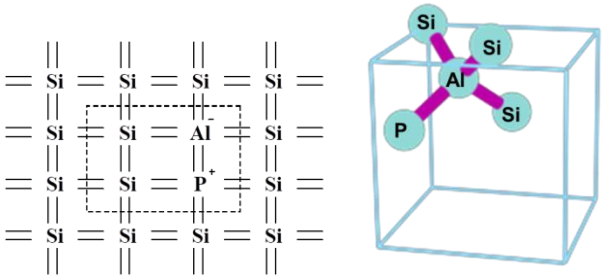

Fig. 1 – Heterostructure with unit cells of the type $Si_2A^{III}B^{V}$ in the silicon lattice

According to [6-7], for the formation of such unit cells it is necessary to fulfill a number of conditions:

1) The sum of the covalent atomic radius of atoms of groups III and V should not differ significantly from the sum of two covalent silicon atoms:
2) The sum of the valence electrons of these impurity atoms must be equal to 8.
3) The electronegativity of atoms of groups III and V should not differ significantly from the electronegativity of silicon atoms.
4) Atoms of groups III and V in the silicon lattice should be located close enough.
5) It is necessary to select the optimal conditions for sequential diffusion doping, taking into account the diffusion coefficients of atoms of groups III and V, so that the concentration distribution of these impurity atoms coincides as much as possible [8].

Our analysis and calculations taking into account the physical and chemical, as well as diffusion parameters of elements of group III and V in silicon, showed that the pairs BP, AlP, GaP, BSb, GaSb, GaAs are most suitable [7-8]. As the concentration of introduced impurity atoms of groups III and V increases, the probability of the formation of various types of binary unit cells of $Si_2A^{III}B^{V}$ in the silicon lattice (Fig. 2) increases significantly.

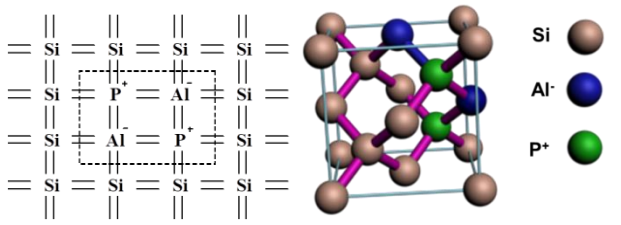

Fig. 2 – Heterostructure with unit cells of type $A^{III}B^{V}$ in a silicon lattice.

At higher concentrations of impurity atoms in the crystal lattice, it becomes possible to form III-V semiconductor compounds on the basis of such unit cells of local nanocrystals (Fig. 3). The solubility of impurity atoms of groups III and V can reach $10^{20} – 10^{21}$ cm^{-3}, while the distance between atoms of groups III and V is 1 – 3 nm, which ensures the formation of nanoclusters of $A^{III}B^{V}$ semiconductor compounds and various associations based on $Si_2A^{III}B^{V}$ unit cells in the crystal lattice silicon.

The size, structure, and concentration of the emerging nanocrystals of III–V semiconductor compounds are mainly determined by the thermodynamic conditions of doping. As the results of the study showed, for the formation of unit cells and their associations, it is necessary to conduct additional thermal annealing at lower temperatures than the diffusion temperature after diffusion doping [9-10].

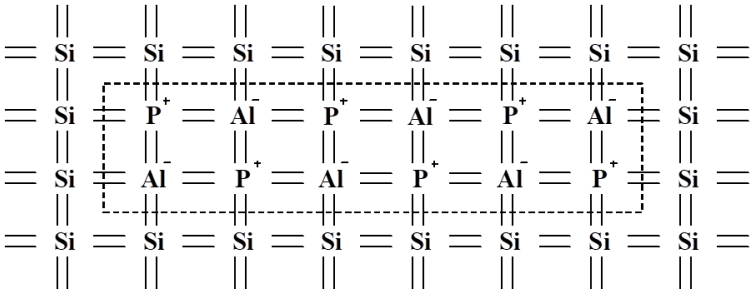

Fig. 3 – Heterostructure with $Al^{-}P^{+}$ ($A^{III}B^{V}$) nanocrystals in a silicon lattice

The temperature and time of additional thermal annealing depends on the electrophysical, chemical, and diffusion parameters of impurity atoms of groups III and V. It was established that, depending on the nature of the impurity atoms of groups III and V, the temperature of additional thermal annealing is in the range from 650 to 1000 °*C* with an annealing time of 2 to 10 hours.

In contrast to the silicon crystal lattice, new $Si_2A^{III}B^{V}$ unit cells are being formed that have an ion-covalent bond; therefore, the necessary energy for the release of electrons from these unit cells (i.e., the energy of the band gap) will differ significantly from the energy of the band gap of pure silicon. Depending on the structure and composition of the unit cells, it can be more or less than the energy of the band gap of silicon.

For nanocrystals formed in the silicon crystal lattice, the energy of the band gap will be close to the corresponding energy of the III – V semiconductor compound. On the other hand, the various associations of binary cells based on $Si_2A^{III}B^{V}$ and $A^{III}B^{V}$ nanocrystals formed in the silicon lattice act as quantum dots that change not only the energy state of electrons, but can also create energy minibands [11].

At a sufficiently high doping level, each of the unit cells, their associations, and nanocrystals will make a significant contribution to the absorption of light in the UV, visible, and IR spectral regions, i.e. an almost new silicon-based semiconductor material with an expanded spectral sensitivity region is obtained.

The formed local $A^{III}B^{V}$ nanocrystals of various sizes in the silicon lattice should have an energy band structure corresponding to III-V semiconductor compounds, i.e. a local nanoscale site with a direct-gap structure appears. This means that a local region with high emissivity appears in the crystal lattice of silicon.

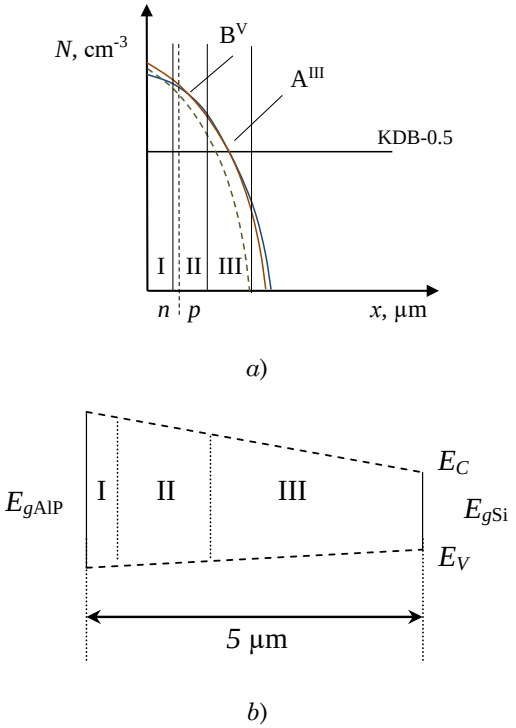

Fig. 4 – The structure of the $A^{III}B^{V}$ – Si heterostructure in the silicon lattice. a) enriched regions of nanocrystals and unit cells, b) is the band diagram of the AlP – Si heterostructure

Thus, choosing the optimal pairs of atoms of elements of groups III and V, as well as determining the optimal conditions for doping and the formation of binary unit cells with the participation of elements of groups III and V, one can control the basic fundamental parameters of silicon, i.e. Based on silicon, it is possible

to create a new material with the necessary fundamental parameters, which can have unique electrophysical, photoelectric, optical and magnetic properties and other functionalities that not only silicon, but also the III-V semiconductor compounds themselves do not have. This means that such materials in the future can replace the unique, but very expensive semiconductor compounds $A^{III}B^{V}$ and even $A^{II}B^{VI}$.

Preliminary results of the study showed that doping of silicon with impurity atoms of groups III and V under optimal thermodynamic conditions forms a near-surface region 5 – 6 μm thick consisting of several separate regions (Fig. 4) (this value can be changed by changing the diffusion conditions). The first region 0.1 – 0.5 μm thick is enriched with $A^{III}B^{V}$ nanocrystals, followed by the second region 0.5 – 2 μm thick enriched with associations of $A^{III}B^{V}$ unit cells, then the third region is 2 – 5 μm thick enriched with $Si_2A^{III}B^{V}$ unit cells, followed by silicon substrate (Fig. 4).

3. EXPERIMENTAL

For fabrication of silicon samples with $A^{III}B^{V}$ compounds using the low-temperature gradual diffusion [12], we use single-crystalline silicon with p-type conduction and resistivity of $\rho = 0.5$ Ω cm. The doping temperature was chosen at 1200 °C to obtain the maximum solubility of phosphorus and aluminum introduced into silicon. Initially, silicon was doped with phosphorus for 8 hours, then aluminum was diffused for 5 hours. The temperature of additional thermal annealing was 800 °C with an annealing time of 4 hours. After the diffusion process, the samples were chemically treated in hydrofluoric acid (HF) to remove aluminum and phosphorosilicate glass from the front surface.

To practically confirm the formation of $A^{III}B^{V}$ compounds in the silicon crystal lattice by X-ray energy dispersive and X-ray diffraction analysis, in order to exceed the sensitivity threshold of these methods, sequential diffusion of phosphorus and aluminum into single-crystal silicon was carried out, which ensured the highest concentration of the resulting $A^{III}B^{V}$ compound.

4. RESULTS AND DISCUSSION

The elemental composition of the surface of Si (Al+P) samples was studied using an EVO MA-10 scanning electron microscope with an X-ray microanalysis mode. The results of X-ray energy dispersive microanalysis of the obtained clusters are shown in Fig. 5 (spectrum 35 and spectrum 37). As can be seen from the obtained results, Al and P have an equal percentage of about 2 %, which indicates the formation of the AlP compound and corresponds to a concentration of introduced elements of 10^{21} cm $^{-3}$. It should be noted that similar results were observed over the entire surface of the samples, as well as the fact that the AlP compound is rapidly destroyed in the air atmosphere and can be present in the stable state only in the bulk of silicon.

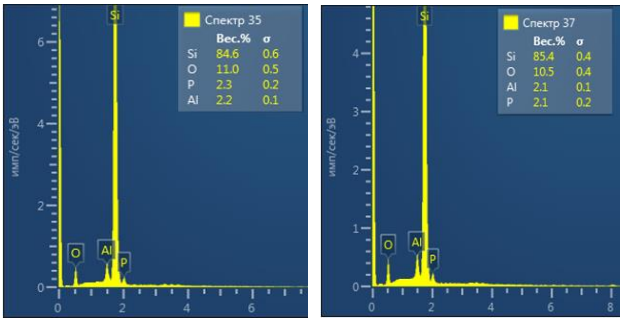

Fig. 5 – Theresults of X ray energy dispersive microanalysis of the obtained binary AlP clusters (spectrum 35 and spectrum 37)

Further, the obtained samples were subjected to X-ray diffraction analysis. The results of X-ray diffraction analysis of Si (Al + P) are shown in Fig. 6. As can be seen from the obtained results, the probability of coincidence for the AlP crystal structure is more than 99 %, for $AlPO_4$ and $AlSiP_3$ structures less than 1 %.

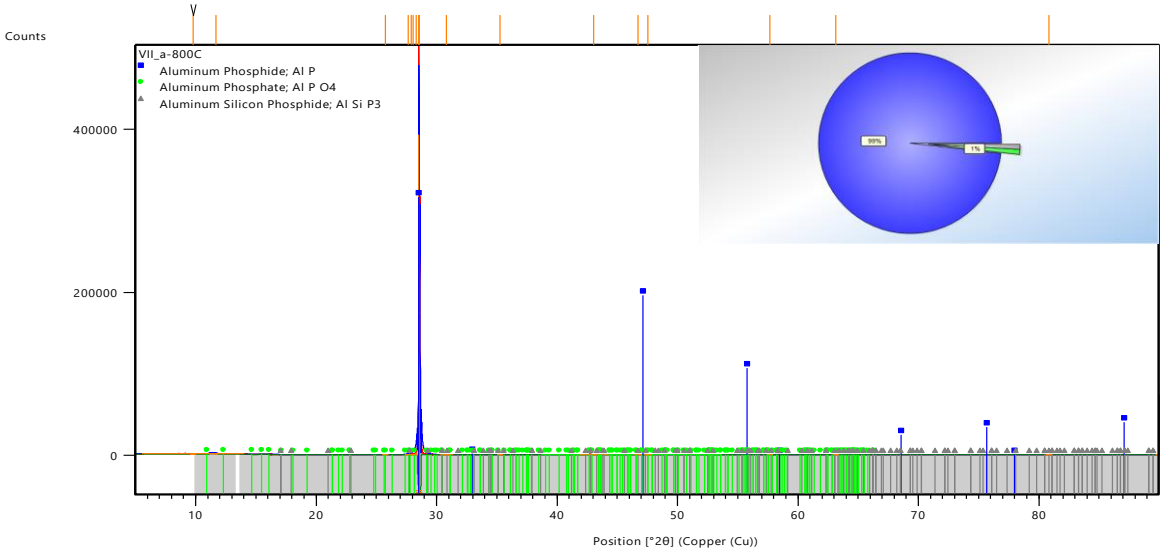

Fig. 6 – Results of X-ray diffraction analysis of the obtained binary AlP clusters

5. CONCLUSIONS

As the results of the study showed, with an increase in the concentration of introduced impurity atoms, molecules are associated with the formation of more complex structures, which at the end form the nuclei of a new phase of the semiconductor compound. In this case, the formation of nanocrystals of semiconductor compounds AlP and Si_2AlP in the crystal lattice of silicon creating burial heterostructures. We hope that the improvement of the technological processes of cluster formation and the implementation of more detailed theoretical calculations will make it possible in the future to more accurately control the formation of heterostructures based on $Si_2A^{III}B^{V}$ unit cells in a silicon crystal lattice.

ACKNOWLEDGEMENTS

We would like to express our sincere gratitude to our supervisor, Professor, Academician Mukhamed Kabir Bakhadirkhanov, for his valuable guidance and support throughout the research process.

This work was financially supported by Science and Technology projects PROJECT PROPOSAL FOR UZBEK-CHINA RESEARCH PROGRAM,"National Key R&D Program of China",№:2016YFE0120900.

REFERENCES

1. Zh.I. Alferov, *Scientific Session of the General Meeting of the Russian Academy of Sciences* **81** No 3, 197 (2011).
2. M.G. Mil'vidskii, V.V. Chaldyshev, *Semiconductors* **32** No 5, 457 (1998).
3. M.K. Bakhadyrkhanov, S.B. Isamov, S.A. Tachilin, N.F. Zikrillaev, *Appl. Sol. Energy* **48** No 1, 55 (2012).
4. M.K. Bakhadyrkhanov, S.B. Isamov, Kh.M. Iliev, S.A. Tachilin, K.U. Kamalov *Appl. Sol. Energy* **50** No 2, 61 (2014).
5. Y. Hu, C. Qiu, T. Shen, K. Yang, H. Deng, *J. Semiconductors* **42**, 11 (2021).
6. S.Z. Zainabidinov, A.S. Saidov, M.U. Kalanov, A.Y. Boboeva, *Appl. Sol. Energy* **55** No 5, 291 (2019).
7. J. Emsley, *Oxford University Press* **296** (1997).
8. A. Mostafa, M. Medraj, *Materials* **10**, 676 (2017).
9. N.B. Uner, E. Thimsen, *J. Phys. D: Appl. Phys.* **53**, 095201 (2020).
10. Mazur, B.R.T.M.T.W.E., *Applied Physics A: Materials Science & Processing,* **96** No 2, 4 (2009).
11. S. Kumar, D.K. Aswal, *Materials Horizons: From Nature to Nanomaterials* 721 (2020).
12. M.K. Bakhadyrkhanov, Z.T. Kenzhaev, S.V. Koveshnikov, A.A. Usmonov, G.Kh. Mavlonov, *Inorganic Materials* **58**, 1 (2022).

Нове технологічне рішення для створення багатошарових систем на основі кремнію з бінарними нанокластерами та елементами III та V груп

N.F. Zikrillayev[1], S.B. Isamov[1], B.O. Isakov[1], T. Wumaier[2], Li wen Liang[2], J.X. Zhan[2], T. Xiayimulati[2]

[1] *Tashkent State Technical University, 100095 Tashkent, Uzbekistan*
[2] *Xinjiang Institute of Engineering, 830023 Urumchi, China*

Розроблено дифузійну технологію формування бінарних кластерів в кремії за участю елементів III і V груп. Показано, що шляхом контролю концентрації елементів атомів III і V групи можна сформувати багатошарові гетропереходи на основі кремнію в поверхневій області кремнію зі збагаченими нанокристалами AIIIBV, а потім збагаченими різними комбінаціями елементарних комірок Si2AIIIBV (1 – 5 мкм товщиною). Це створює практичний новий матеріал на основі кремнію - безперервну варизонну структуру завдяки плавному переходу від забороненої зони напівпровідникових сполук III – V до забороненої зони кремнію.

Ключові слова: Напівпровідник, Бінарні кластери, Елементарні клітини, Самоорганізація, Самоструктура, Наноструктура, Нанокристал, Світлочутливість, Комбінації, Багатоступеневі фотоелементи.