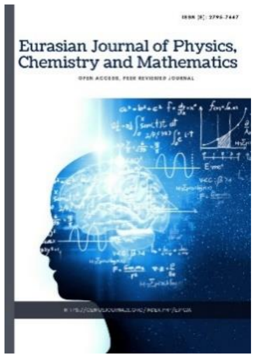


Electrophysical properties of single-crystal silicon sequentially doped with sulfur and zinc impurity atoms

M.K. Haqqulov Tashkent state technical university.

ABSTRACT

The paper studies electro physical properties of single crystal silicon after gradual (first-sulfur, afterwards -zinc) diffusion of impurity atoms of sulfur and zinc. The authors investigated how the Si_2ZnS -structured binary compounds form in the crystal lattice of silicon and also studied the physical mechanisms of how additional thermal treatment might influence the process of formation of clusters.

Keywords: silicon, zinc, sulfur, cluster, impurity, atom, binary compound, diffusion, concentration

Introduction

Over the past years, researchers in many laboratories around the world have been conducting scientific research aimed at developing a technology for the design of clusters consisting of atoms of two or more elements in the crystal lattice of silicon. At the same time, self-assembly of clusters of binary elements, a thorough knowledge of the physical nature of the mechanism, and the design of a technology for the formation of clusters of nanosized impurity atoms in the crystal lattice of semiconductor materials are of greater importance than ever in harnessing limits of electronics [1–3].

Currently, various modern methods and technologies are being devised that make it possible to engineer and study the composition of nanoscale structures of compounds of various elements in semiconductor materials. Substantial efforts are being made to control their concentration.

Targeted change in the key electrophysical parameters of semiconductor materials based on controlling the concentration of various compounds, as well as building tunable concentration of nanosized compounds on the surface and in the bulk of semiconductor materials remains an urgent priority for the electronics industry.

Samples and Research methods

The sequential diffusion process of impurity atoms into silicon was carried out as follows. At the first stage, samples of *n*-type conductivity single-crystal silicon (phosphorus doped silicon-100) were prepared, together with impurity of sulfur (S). They were placed in quartz ampoules and that were vacuumized (P=10^{-5}÷10^{-6} mm. Hg). Quartz ampoules were placed into a diffusion furnace at room temperature T=300°K.

Then the furnace was heated to the temperature T_{min}=550°C gradually at 5 deg/min increments and kept at this temperature for a certain period of time t_1. Afterwards, the temperature in the furnace was increased to the required maximum T_{max} =1250°C and kept at this temperature for time t_2. Having finished the diffusion process, the quartz ampoules were removed from the furnace and immediately cooled. During the diffusion process, it was found that the diffusion parameters depend on temperature values of T_{min} and T_{max} (minimum and maximum), the exposure time at a given temperature as well as the concentration of phosphorus atoms in the initial sample. At the second stage, the diffusion of zinc impurity atoms into silicon samples doped with sulfur (S) was carried out by implementing a traditional high-temperature diffusion technology.

In this case, *n*-type conductivity silicon samples (phosphorus-doped silicon -100) doped with sulfur (S) were placed together with zinc (Zn) impurity into quartz ampoules, the ampoules were vacuumized (P=10^{-5}÷10^{-6} mm. Hg) and put into the furnace. The process of diffusion of zinc impurity atoms was carried out at a temperature T_{max}=*1200°C* and for a certain period of time *t*. After completion of the diffusion process, the quartz ampoules were taken out of the furnace and quickly cooled. In parallel and as a reference case, the diffusion of zinc (Zn) impurity atoms into the starting silicon sample was also carried out using high-temperature diffusion technology.

In this case, the samples of *n*-type silicon (phosphorus-doped silicon -100) with zinc (Zn) impurity were placed in quartz ampoules, air was pumped out, and together with quartz ampoules, in which sulfur atoms were diffused into silicon, they were placed into an electric furnace after the temperature of diffusion was set in it and shortly thereafter the diffusion was initiated.

The concentration dependence of the depth of penetration of zinc impurity atoms into a silicon single crystal after the diffusion process is shown in Figure 1.

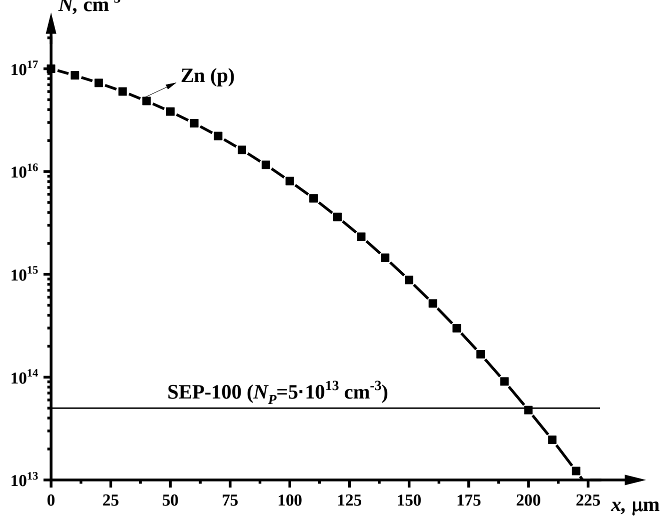


Fig.1. Concentration versus the penetration depth of zinc impurity atoms into a single crystal silicon sample

The analysis of the above experimental results was carried out by comparing the basic electrical parameters of silicon samples after the sequential diffusion process has ended. The bulk and surface fundamental electrophysical parameters of silicon samples, in which zinc and sulfur atoms were embedded, were determined using *Ecopia HMS-3000 Hall instrument* and a conductive-type thermal probe (*n* or *p* type). In this case, the order of gradual decrease in the concentration of impurity atoms was studied by layer-by-layer destruction of the surface of silicon samples of the Si<Zn> and Si<ZnS> structures.

On Figure 2a and 2b the distribution of sulfur and zinc impurity atoms in single-crystal silicon after successive diffusion are shown, as well as the formation of Si_2ZnS-structured binary compounds.

a

b

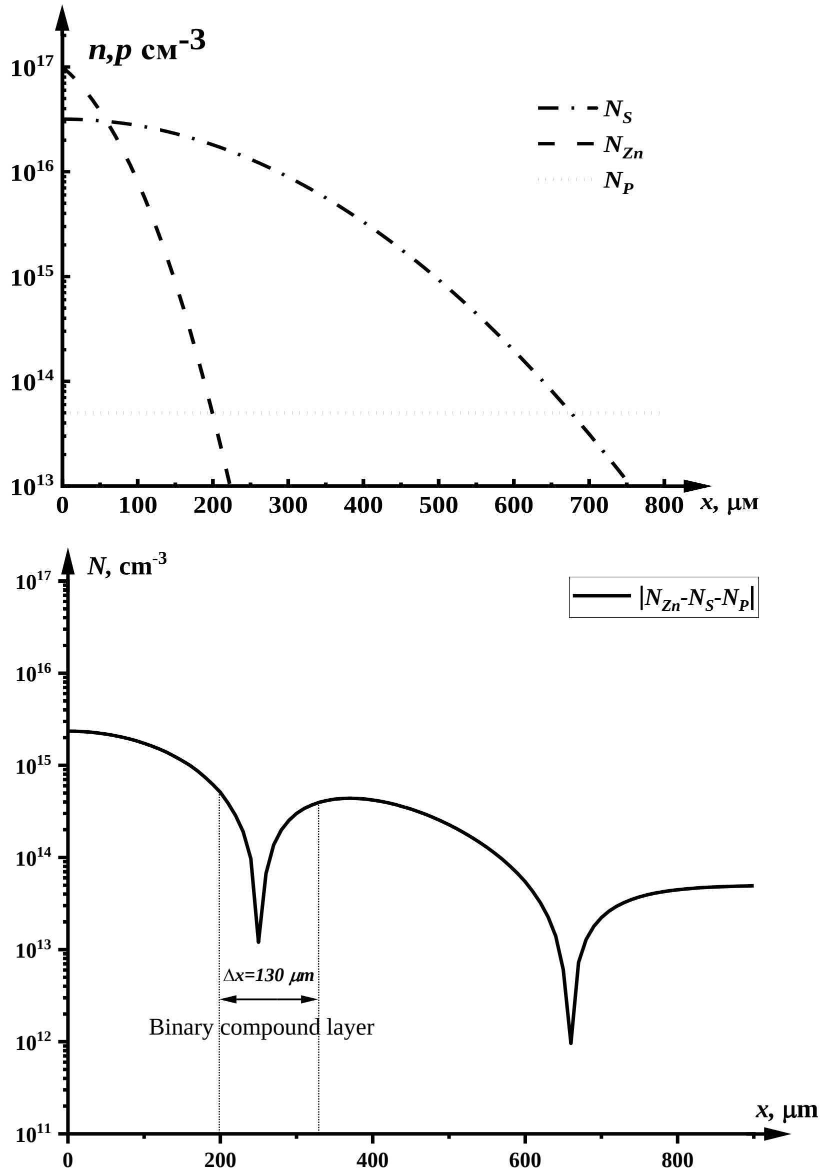


Fig.2 a) bulk distribution of Si_2ZnS-structured binary compounds in single- crystal silicon, b) formation of a layer of Si_2ZnS-structured binary compounds on the surface of single-crystal silicon

At the third stage, additional thermal treatment was performed in order to increase the concentration of Si_2ZnS-structured compounds of the in the bulk of silicon sample. Additional thermal treatment was carried out at *T*=850^{0}C for *t=1 hour*. In this case, preconditions were created for that ensure building of mutually neutral compounds between zinc atoms (which became doubly charged positive ions) and sulfur atoms (which became doubly charged negative ions) (Fig.3). As can be seen from Figure 3, it was observed that the layer of formation of binary compounds expanded twice, that is, their concentration distribution across the bulk had increased.

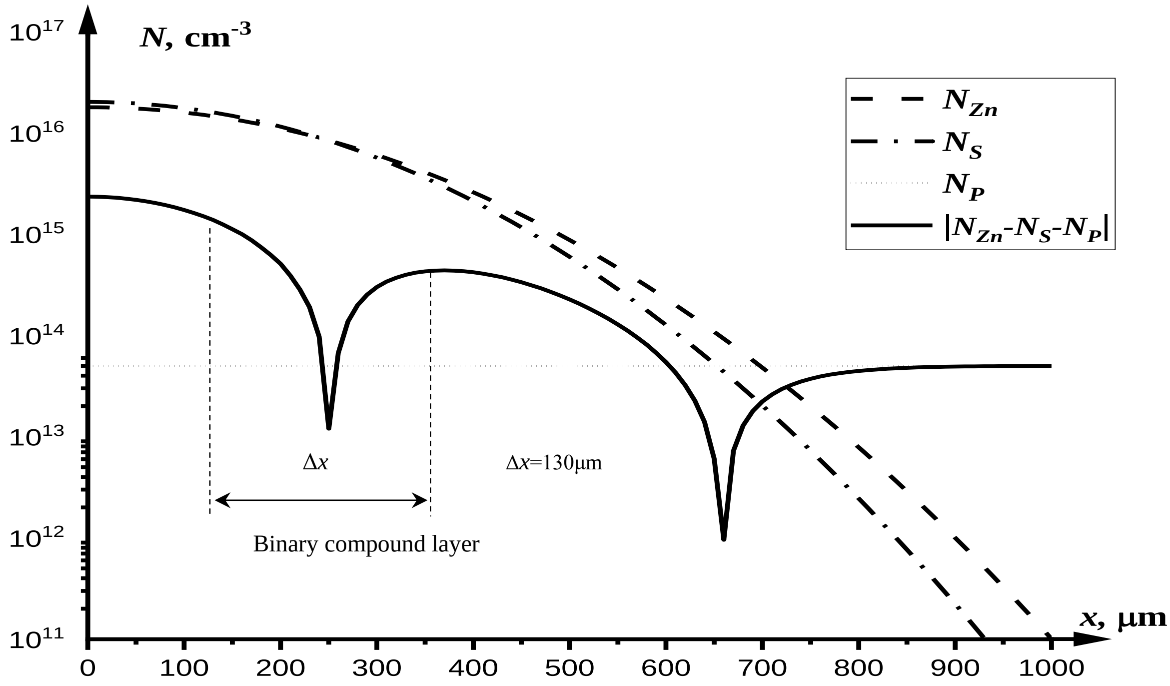
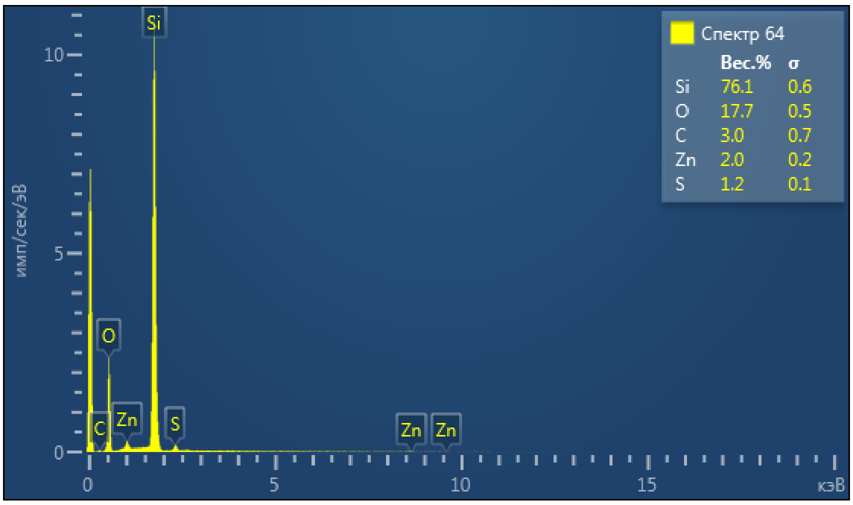


Fig. 3. Depth of ZnS after additional thermal treatment of the silicon samples

The study and elemental analysis of the surface of heat-treated silicon samples was carried out using a *SEM-EVO MA 10 type scanning electron microscope* (Fig. 4). The results of the analysis of the elemental composition of the silicon surface showed that, in terms of mass, it consists of: 76.1% silicon atoms, 17.7% oxygen atoms, 3% carbon atoms, 2% zinc atoms, 1.2% sulfur atoms.



Element	Weight %	σ. %
Si	76.1	0.6
O	17.7	0.5
C	3.0	0.7
Zn	2.0	0.2
S	1.2	0.1
Total:	100.00	

Fig. 4. Elemental composition of $Si_2Zn^{--}S^{++}$ compounds in single-crystal silicon surface

Additionally, thermally treated at T=850÷875^0C for t=0.5÷2 hours, silicon samples with Si_2ZnS-structured compounds in the bulk must have naturally undergone changes in their structure. In order to reveal such structural changes in samples, further XRD analyzes may well shed light on such structural changes.

One can assume that as a result of sequential gaseous diffusion of sulfur and zinc into silicon, Si_2ZnS-type structures may well have been formed in the bulk of the crystal

Conclusion

Summarizing the above the experimental results and based on the analysis of behavior of various elements in silicon, one can assume that the sequential (two-stage) diffusion of sulfur and zinc atoms into silicon might result in building of $Si_2Zn^{--}S^{++}$ -type new compound in the bulk of the material.

The results of the experiments showed that a new crystal structure containing ZnS-type bonds on the Si surface and in the bulk can be formed using an inexpensive and widely used diffusion doping technology. Therefore, today substantial scientific and practical interest is drawn to the study of the effect of binary compounds on the crystal lattice, leading to a substantial alteration in the properties of silicon that could be used for the design of novel materials for optical electronics, solar cells and e.t.c.

References

1. John McCloy and Randal Tustison. Chemical vapor deposited zinc sulfide, Published by SPIE The International Society for Optical Engineering P.O. Box 10 Bellingham, Washington USA, - 2013.- P. 1-9.
2. Bakhadirkhanov M. K., Mavlyanov A., Sodikov U., Khakkulov M. Silicon with Binary Elementary Cells as a Novel Class of Materials for Future Photoenergetics// ISSN 0003_701X, Applied Solar Energy, 2015, Vol. 51, No. 4, pp. 258-261. Allerton Press, Inc., 2015.
3. N.F.Zikrillaev, F.Q.Shakarov, M. K. Khaqqulov. Numerical calculation of the charge state and electrostatic potential of a binary nanocluster structure with Si2ZnS cells in a cubic lattice of crystalline silicon with a diamond structure. Technical science and innovation, Vol.10 (2020): Iss. 3, Article 12.
4. Н.В. Ганина. Физико-химические особенности изовалентного легирования полупроводников. Physics and Chemistry of Solid State. V. 3, № 4 (2002) P. 565-572.
5. Joongoo Kang, Ji-Sang Park, Pauls Stradins, and Su-Huai Wei. Nonisovalent Si-III-V and Si-II-VI alloys: Covalent, ionic, and mixed phases. Physical Review B, 2017. Volume 96; Issue 4, 045203.
6. Zikrillaev N.F., Koveshnikov S.V., Isamov S.B., Abdurahmonov B.A., Kushiev G.A. Spectral dependence of the photoconductivity of Ge xSi1 – x type graded-gap structures obtained by diffusion technology. Semiconductorsthis link is disabled, 2022, 56(1), pp. 29–31
7. Мильвидский М.Г., Чалдышев В.В. Наноразмерные атомные кластеры в полупроводниках - новый подход к формированию свойств материалов. Физика и техника полупроводников, 1998, том 32, № 5. С.513-522.
8. Bakhadirkhanov, M.K., Ibodullaev, S.N., Zikrillaev, N.F., Koveshnikov, S.V. An Infrared Radiation Photoresistor Based on Silicon with Nanoclusters of Manganese Atoms. Technical Physics Lettersthis link is disabled, 2021, 47(9), pp. 641–644.
9. А.Т. Лончаков. О природе низкотемпературной аномалии динамических модулей упругости в кубических кристаллах $A^{II}B^{VI}$ с примесями 3d-переходных металлов. Физика низких температур, 2011, т. 37, № 4, с. 450–455.