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Binary Compounds in Silicon Bulk and their Impact on Parameters of Silicon

Khakkulov M.K

PhD student ,Department of Electronics and Microelectronics, Tashkent State Technical University, 100095, Tashkent, Uzbekistan

ABSTRACTThe author counducted diffusion doping of Cd and S in Si. Originally the authors had chosen p-type Si sample with ρ = 5 Ω·см (concentration of holes $p=7\cdot10^{15}см^{-3}$). The report shows that Increasing concentration of binary compounds in silicon matrix would have allowed us to change some parameters of basic silicon material and use it for various purposes such as more efficient photocells for example. STM analysis would have allowed us to investigate and confirm that lattice parameters in silicon in lattice sites where Si atoms were replaced by Cd and S must have changed and we are currently on our way to study these properties

I. INTRODUCTION

In silicon samples with nanoclusters of manganese atoms we have been able to observe some very interesting physical phenomena. In the course of study of magnetic properties of these materials, we have been able to discover anomalously large negative magneto-resistance (NMR) at *T = 300 K* [1,2], i.e. the ferromagnetic state of silicon [3]. Magnetic properties can be varied over a wide range by means of temperature, electric field, and irradiation [4,5]. We have also been able to reveal double inversion of the value of the magneto-resistance (MR) [4,5]. Meanwhile, in the course of study of photovoltaic properties, we had revealed bias of the photo-response edge towards λ = 10 micron, an anomalously high impurity photoconductivity in the diapason *λ = 10 ÷ 1,5 micron* [6,7], as well as the effect of the stimulated impurity photoconductivity in the presence of background light.

II. EXPERIMENT

One of the solutions in modern photovoltaics aimed at reducing the thermalization effect and increasing the absorption coefficient of the UV and visible part of the solar spectrum is based on semiconductor compounds type -$A^{III}B^{V}$ (multistage photocells) [1].

Multi-cascade photocells are characterized by high performance, however the technology of their production is rather complex and requires expensive equipment. Therefore, such solar cells have a high cost. At the same time, their widespread terrestrial application is not well developed.

Therefore, of great scientific and practical interest is the idea of formation in the crystal lattice of Si of clusters of impurity atoms, in particular the binary clusters of impurity atoms representing a kind of new elementary cell type- $Si_2A^nB^{8-n}$ (where A and B - impurity atoms that replace the neighboring lattice sites Si and n - number of valence electrons).

Meanwhile, the following conditions must be in place in order to shape such elementary cells in the silicon lattice:
1) The sum of valence electrons of atoms A and B must be equal to 8 so that in case of substitution of 2 neighboring silicon atoms in the lattice, the tetrahedral partially ion-covalent bond in the silicon lattice is not compromised.
2) One of the impurity atoms of A or B must have a sufficiently high diffusion coefficient, i.e. it should preferably move by the interstices mechanism, to increase the probability of formation of a compound $A^{-m}B^{+m}$.
3) Both impurity atoms should have sufficient chemical activity that would ensure the existence in nature of these compounds $A^{-m}B^{+m}$.

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Such elementary cells not only have their own fundamental parameters like band-gap, mobility, and the dielectric constant and the lattice parameter, but also represent a kind of a quantum dots that provide quantum mechanical features on such nanostructures.

By selecting elements of these groups based on the values of the electro-negativity, the size of atoms, solubility and diffusion coefficients, it could be possible to form the elementary cells type « $Si_2A^nB^{8-n}$ - quantum dots" in the Si lattice with controlled fundamental parameters, which would contribute to the generation of photocarriers for $hv<E_g$ and $hv>E_g$. This will significantly expand the spectral range of silicon sensitivity.

Of particular interest is the development of technology for the formation of such elementary cells - nanostructures of different nature, and controlling their concentration in the silicon lattice[2].

The main feature of such structures are ideal current-voltage characteristics due to lack of surface states, which are always present in all modern such structures.
We have developed a technique of low-temperature impurity doping of silicon by atoms A and B either sequentially or simultaneously, which ensures maximum participation of atoms involved in the formation of compounds. The optimal technological and thermodynamic conditions for the formation and controlling parameters of the mono-atomic and binary clusters of impurity atoms depending on their electrical, chemical and diffusion parameters of impurity atoms in silicon are defined. Unlike existing methods of forming nanostructures (MBE), this processing method is not only quite convenient in use and is relatively inexpensive, but also allows quantum dots to form uniformly throughout the bulk.

We have comprehensively analyzed the possibility of forming such bands between the elements of Group II and transition elements with the elements of Group VI.

The results of electrical measurements of the samples studied show that in silicon samples doped with manganese conductivity type has become the n-type to $\rho \sim 2\div3\cdot10^3$ Ω·см, and silicon samples doped with sulfur also become n-type with $\rho \sim 0{,}3$ Ω·см. These data indicate that these impurities in silicon are donors[3]. Therefore, it can be assumed that the silicon is simultaneously doped with Mn and S, should be a low-resistance n-type material. However, the results showed that they were a high-resistance n-type materials, i.e., as the concentration of these impurities in the samples was reduced significantly. Studies using activation analysis showed that in the samples, the concentration of Mn and S atoms is the same as in the silicon sample doped with manganese and sulfur separately. Therefore, it can be assumed that in Si <B, Mn, S> samples interaction occurs between Mn atoms and S.

The authorscounducted diffusion doping of Cd and S in Si. Originally we had chosen p-type Si sample with $\rho = 5$ Ω·см (concentration of holes $p=7\cdot10^{15}$ см$^{-3}$). We conducted diffusion for 12 hours simultaneously of Cd and S in a single closed ampoule with vacuum 10^{-5}mm of mercury column in furnace at temperature T=1200 ^{0}C. While temperature steadily increased we at temperature 700^{0}C stopped for a while (30 minutes) with assumption that Cd and S could eventually actually form binary compound in the Si matrix. After having reached 12 hours we instantly cooled off the ampoule in transformer oil to fix the compounds in the matrix. We carried out the Hall effect measurements of the mobility of charge carriers and determined conductivity. The sample dimensions were d=0,083cm, a=0,377 cm, l=0,27 cm.
The results of electro-physical measurements are given in Table 1 and 2.

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Table 1

	+	-
U_{SN}	27 mV	39,1 mV
U_{NS}	19,5mV	32,3 mV
U_0	22mV	37 mV
U_δ	1,4V	1,1 V
I	2,67mA	1,58 mA

Table 2

U_H	3,5755 mV
R_H	$9{,}977 \cdot 10^3$ Ω
ρ	68,2 Ω·см
μ_δ	146,31 $cm^2/V \cdot s$
p	$6{,}27 \cdot 10^{14}$ $см^{-3}$

The results of electro-physical measurements in Table 1 and Table 2

III. CONCLUSION

As we know, S predominantly gives donor type levels in silicon while Cd in lattice site forms mainly tetrahedral bands with silicon as acceptor. We assume that S and Cd in silicon must have formed tetrahedral band with silicon matrix and with each other since its concentration of holes decreases slightly after diffusion from $p=7 \cdot 10^{15} см^{-3}$ to $p=6{,}27 \cdot 10^{14} см^{-3}$ while conductivity increases from 5 Ω·см to 68,2 Ω·см.

Increasing concentration of binary compounds in silicon matrix would have allowed us to change some parameters of basic silicon material and use it for various purposes such as more efficient photocells for example. STM analysis would have allowed us to investigate and confirm that lattice parameters in silicon in lattice sites where Si atoms were replaced by Cd and S must have changed and we are currently on our way to study these properties.

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