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REGULAR ARTICLE

The Prospects of Obtaining a New Material with a Hetero-Baric Structure Ge$_x$si$_{1-x}$–Si Based on Silicon for Photo Energy Applications

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This study defines the technological procedures for obtaining Ge$_x$Si$_{1-x}$ alloys through the diffusion method by introducing germanium atoms into monocrystalline silicon. The research results indicate that the fundamental parameters of the resulting Ge$_x$Si$_{1-x}$ alloys differ from the fundamental parameters of the initial silicon, particularly altering the energy values of silicon's forbidden zone. Elemental analysis of the sample surfaces revealed silicon concentration (in atomic percentages) of approximately ~ 70.66 % and germanium ~29.36%. To manufacture and study the parameters of silicon-based solar cells with Ge$_x$Si$_{1-x}$–Si heterostructures, we used samples obtained by two different methods. In the first method, the *p-n* junction was formed by introducing phosphorus impurity atoms into the original silicon of *p*-type silicon grade. In the second method, the *p-n* junction was formed by boron diffusion into the original silicon of SEPH (silicon electronic type, doping material of phosphorus) grade. In both cases, the depth of the *p-n* junction ranged from 0.5 to 6 μm. It was also shown that the binary compounds Ge$_x$Si$_{1-x}$ are a new material for modern electronics; the possibility of creating properties in electronics based on them was shown. Based on them, it is proposed to create devices and new functionality and highly efficient solar cells.

Keywords: Diffusion, Germanium, Silicon, Manganese, Heterostructures, Elemental Analysis.

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1. INTRODUCTION

Today, special attention is given to the development of new materials with clusters of impurity atoms on the surface and within the volume of a semiconductor, which is one of the primary directions in the technology and physics of semiconductor materials [1-3]. An important task within this context is to create a simple and cost-effective technology for forming clusters of impurity atoms within the crystal volume, allowing the creation of nanoscale structures that alter the properties of the base material. Molecular beam epitaxial methods, used to obtain such nanoscale structures, require expensive equipment. Solid alloys with the Ge$_x$Si$_{1-x}$ combination are produced mainly by liquid-phase epitaxy or gas growth methods, based on the formation of a chemical bond between germanium and silicon elements [4-6]. However, these technological methods do not make it possible to obtain solid Ge$_x$Si$_{1-x}$ compounds of controlled thickness and composition on the surface of single-crystal silicon based on the diffusion method and to form nano-sized cells of the silicon-germanium type in the silicon lattice. diffusion method and to form nano-sized cells of the silicon-germanium type in the silicon lattice.

During solidification, the solid solution of germanium in silicon decomposes, and the excess germanium forms clusters predominantly containing germanium (the solubility of silicon in germanium at 1550 K is less than 50 %) [7].

The aim of this research is to develop a diffusion-based technology for generating germanium clusters within the lattice volume of silicon and to investigate the electrical parameters of these materials.

2. METHODOLOGY

Monocrystalline silicon of both p- and n-types, with resistivity of 10 and 100 Ohm·sm respectively, was chosen as the initial material. The dimensions of all silicon samples were consistent at 8 × 4 × 1 mm^3. Although the diffusion technology for obtaining solid solutions of Ge$_x$Si$_{1-x}$ with various component ratios is of significant interest, it is technologically impractical. This is primarily due to the extremely low diffusion coefficient of germanium atoms in silicon ($D_0 \sim 10^{-14}$ cm^2/s) [5], requiring an extensive diffusion time (Table 1) to achieve layers with high germanium concentration. Here, '*x*' - denotes the depth at which the concentration of germanium drops to '*e*', and the diffusion time is 20 hours.

The issue of the low diffusion coefficient has been resolved through the utilization of low-temperature diffusion doping technology involving silicon and germanium.

3. RESULTS AND ITS DISCUSSION

The two-stage diffusion technology was utilized, enabling a significant increase in diffusion coefficients [3, 6, 7]. Initial silicon samples and the diffusant State Electric Power Station (ГЭС-1) powdered germanium,

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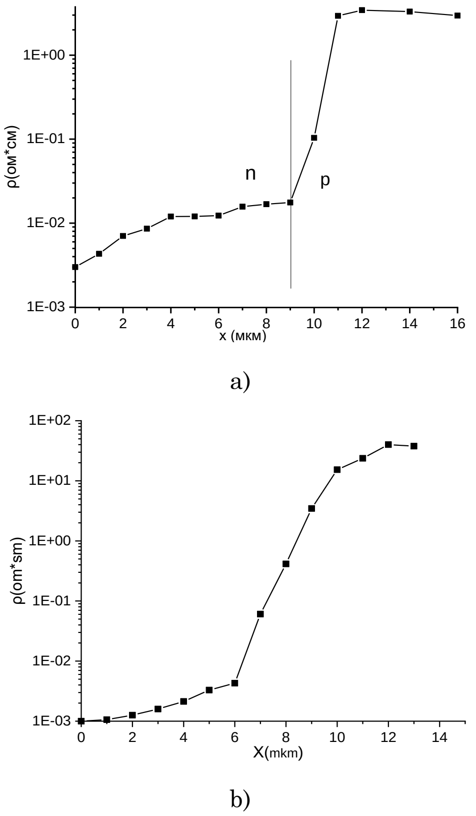
were placed inside quartz ampoules, followed by a vacuum sealing process (residual pressure in the ampoule approximately $P \sim 10^{-5}$ mm Hg). The ampoules were placed in a diffusion furnace of the brand (ВТП) High-Temperature Furnace. 1700 °C at $T = 300$ K

The quantity of the diffusant was determined by calculation, based on the ampoule volume and the required vapor pressure (atom concentration) of the diffusant at the diffusion temperature.

Table 1 – Diffusion coefficient of germanium atoms in silicon at different temperatures

Temperature, °C	1250	1200	1150	1050	950
D, cm²/s	$4\ 10^{-13}$	$8\ 10^{-14}$	6.610^{-15}	$6\cdot10^{-17}$	$7\cdot10^{-19}$
x , mcm	3.6	3.12	2.12	1.42	1.6

The electrical parameters of the samples were measured using the ECOPIA HMS-3000 Van der Pauw setup. Profiles of the distribution of electrical parameters in the samples were investigated using the method of mechanical layer removal (at 1-μm intervals), measurements on the Van der Pauw setup, and subsequent calculation of profiles of resistivity, mobility, and carrier concentration. The chemical composition of individual points on the samples was analyzed using energy-dispersive X-ray microanalysis with the SEM (Scanning Electron Microscope) JSM-IT 200.



a)

b)

Fig. 1 – Variation of silicon resistivity with binary compounds Ge_xSi_{1-x} a) Sample No 2, b) Sample No 3

The results (Fig. 2) of the surface resistance study indicated that after diffusion, the surface resistance of the sample decreased by 5 orders of magnitude, indicating a strong surface layer doping with antimony present in germanium

Raman spectroscopy is a precise method for studying the bonding states and symmetry of impurity atoms in semiconductors. These characteristics are reliant on various local vibrational modes of atoms and molecules forming within the crystalline structure. Additionally, Raman spectroscopy finds wide application in diagnosing diverse structures developed within silicon volume [8-10]. Measurements were conducted using a Raman spectrometer within the spectral range of $100\ \text{sm}^{-1}$ to $3400\ \text{cm}^{-1}$. Spectra were generated using a diode laser with a wavelength of $\lambda = 785$ nm.

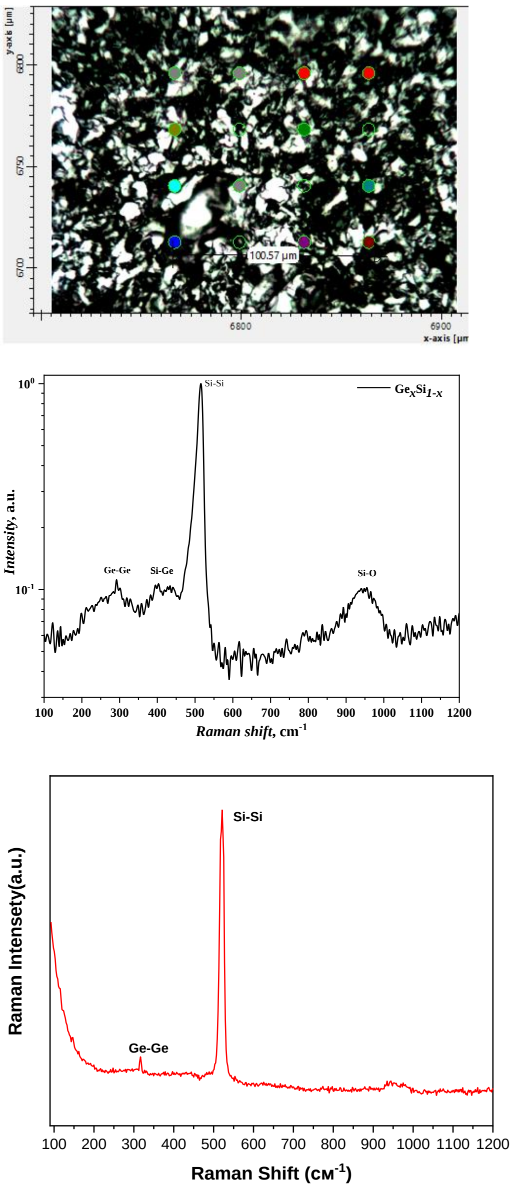
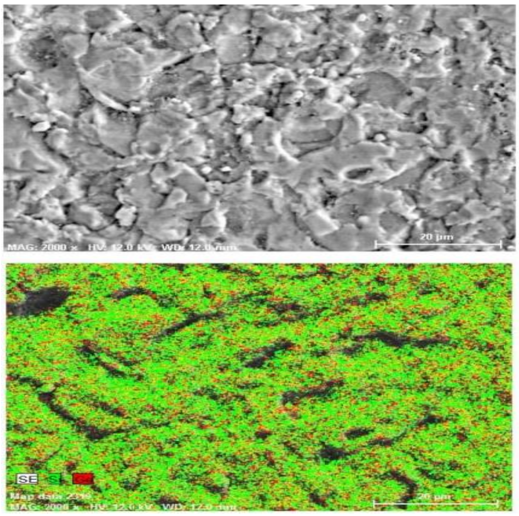
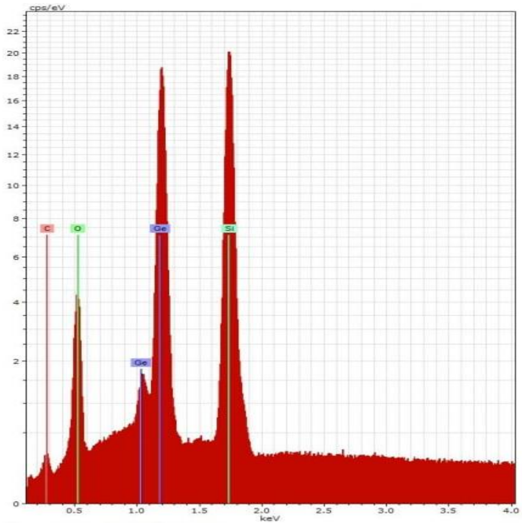


Fig. 2 – Raman spectrum of silicon doped with impurity germanium atoms and annealed silicon sample with Ge_xSi_{1-x} heterostructures ($x \approx 0.27$)

In Fig. 3a, the surface topography of the silicon sample doped with germanium atoms, obtained using SEM (Scanning Electron Microscope) JSM-IT 200 in secondary electron mode, is presented. The X-ray spectrum obtained at point 3 (Fig. 3b) showed that the concentration of silicon atoms was 62 %, and germanium atoms were 38 %, corresponding to the composition of a solid solution $Ge_{0.38}\ Si_{0.62}$.



a)



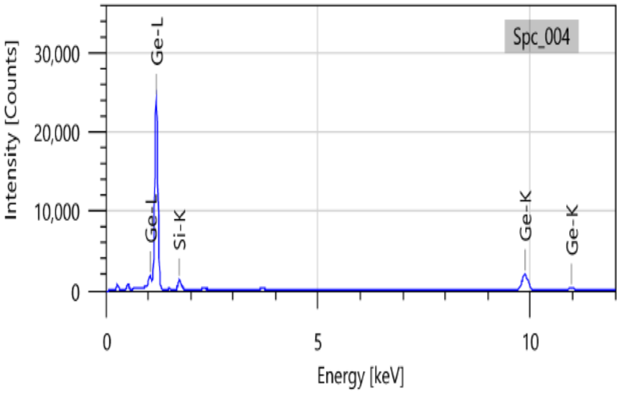
El	AN	Series	unn. C {wt . %}	norm.C {wt . %}	Error {wt . %}
Si	14	K	44.45	44.32	1.8
O	8	K	15.63	15.58	1.9
Ge	32	K	38.23	38.11	2.1
C	6	K	1.99	1.98	0.4
Total:			100.29	100.00	

b)

Fig. 3 – a) Topography of the silicon sample surface after doping with germanium atoms. b) X-ray energy-dispersive microanalysis of silicon samples doped with germanium impurity atoms

From the literature [11-12], it is known that it is impossible to achieve an equilibrium solid solution of germanium in silicon with a germanium concentration exceeding 90 %. The obtained result can be explained by quenching the solution due to the rapid cooling of the samples after diffusion. In Fig. 4, an enlarged image of the sample area near point 4 is shown, along with the elemental composition of the surface.

Judging by the appearance, in this area, there is a droplet of germanium attached to the surface, dissolving a significant amount of silicon. The composition corresponds to a solid solution of silicon in germanium $Ge_{0.87}Si_{0.13}$.



Element	Line	Mass%	Atom %
Si	K	5.59	13. 8
Ge	K	94.41	86.72
General		100.00	100.00

Fig. 4 – Elemental composition of the surface of silicon doped with germanium impurity atoms

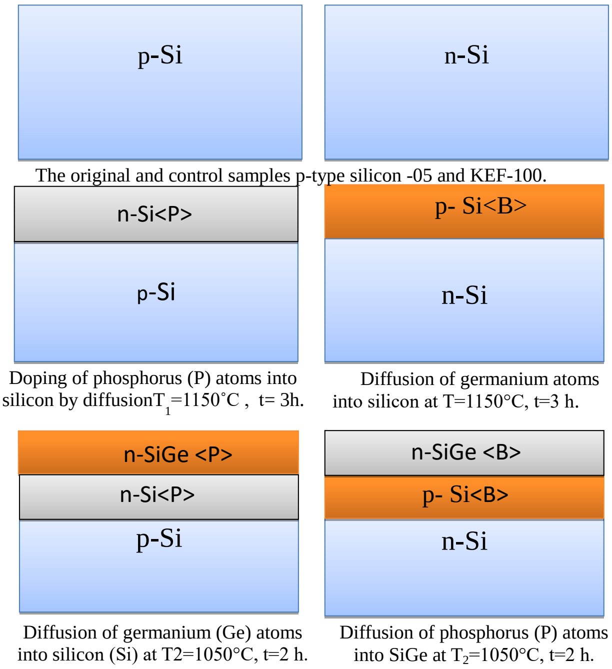


Fig. 5 – Stages of technology for creating a *p-n* junction based on silicon with a heterojunction structure Ge_xSi_{1-x}Si

For the fabrication and investigation of silicon-based solar cells with Ge_xSi_{1-x}–Si heterostructures, samples obtained by two different methods were used [13-16]. In the first method, the *p-n* junction was formed by introducing phosphorus impurity atoms into the original silicon of *p*-type silicon grade. In the second method, the *p-n* junction was formed by boron diffusion into the original silicon of SEPH (silicon electronic type, doping material of phosphorus) grade. In both cases, the depth of the *p-n* junction ranged from 0.5 to 6 μm. Current-collecting contacts of the solar cells were manufactured using the thermal nickel deposition method in a vacuum VUP-5 setup (Vacuum Universal Post). A layer of SiO_2 with a thickness of ~1000 Å was used as an anti-reflective coating. The photovoltaic elements were fabricated in the form of a parallelepiped with dimensions of

2 × 2 cm². Phosphorus diffusion was employed to create *p-n* structures in Si (*p*-type conductivity), forming the front layer of n-type conductivity photovoltaic elements. The structure of the obtained photovoltaic elements based on silicon with the Ge_xSi_{1-x}–Si heterostructure is shown in Fig. 5, using two different methods.

4. CONCLUSIONS

Modifying the fundamental parameters of the original silicon allows for the control of electrical, photoelectric, and optical characteristics of silicon. This enables the creation of a new material with unique photoelectric and optical properties.

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Перспективи отримання нового матеріалу з гетеробаричною структурою Ge_xSi_{1-x}–Si на основі кремнію для застосування у фотоенергетиці

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У даній роботі визначено технологічні параметри та процеси для отримання сплавів Ge_xSi_{1-x} дифузійним методом шляхом введення атомів германію в монокристалічний кремній. Результати досліджень свідчать про те, що параметри отриманих сплавів Ge_xSi_{1-x} відрізняються від параметрів вихідного кремнію, зокрема змінюються значення енергії забороненої зони кремнію. Елементний аналіз поверхонь зразків виявив концентрацію кремнію (в атомних відсотках) приблизно ~ 70,66 % і германію ~ 29,36 %. Для виготовлення та дослідження параметрів кремнієвих сонячних елементів з гетероструктурами Ge_xSi_{1-x}–Si використовувалися зразки, отримані двома різними методами. У першому методі p-n-перехід формувався введенням домішкових атомів фосфору у вихідний кремній p- тип марки кремнію. У другому методі *p-n*-перехід був утворений шляхом дифузії бору у вихідний кремній марки SEPH (кремнієвий електронний тип, легуючий матеріал фосфору). В обох випадках глибина p-n-переходу становила від 0,5 до 6 мкм. Також було показано, що бінарні сполуки Ge_xSi_{1-x} є новим матеріалом для сучасної електроніки; показана можливість формування на їх основі нових електронних пристроїв та функціональних високоефективних сонятних елементів.

Ключові слова: Дифузія, Германій, Кремній, Марганець, Гетероструктури, Елементний аналіз.