Study Of Photocells Based On Ge$_x$Si$_{1-x}$ Stuctures

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The paper presents the results of studying Ge$_x$Si$_{1-x}$ structures obtained using low-temperature diffusion technology. The presence of clusters and their composition in the silicon lattice is determined by electron microscopy and X-ray spectroscopy. The results showed that germanium atoms in the lattice are collected in the form of round islands containing Si$-$ 64.46%, Ge $-$ 26.9%. Between the silicon crystal and the islands there are Ge$_X$Si$_{1-x}$ structures that can affect the photoelectric properties of silicon. It is of interest to study the parameters of solar cells in the presence of such structures. Solar cells containing Ge$_x$Si$_{1-x}$ structures with a p-n junction depth of $6 \div 8\mu$ m on the surface of p-type silicon with $0.5\Omega\cdot$ m were obtained. The concentration of Ge$_x$Si$_{1-x}$ structures was $N \approx 5.610^{19}$ cm^{-3}, while the distance between the island structures was on average 1-2 μm. This distance is much smaller than the distance between the current-collecting contacts. Experiments have shown that the spectral sensitivity of the studied photocells with Ge$_x$Si$_{1-x}$ structures expands toward the infrared region of the solar spectrum. This is explained by the absorption of photons by microheterovariband Ge$_x$Si$_{1-x}$ $-$ Si structures.

Keywords: Photovoltaics; Efficiency, silicon; Renewable energy; Solar cells; Heterovarigated band structure; Diffusion; Germanium

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1. Introduction

Currently, the world is experiencing an increase in demand for energy resources, which in turn requires the expansion of the use of renewable energy sources, in particular solar energy. It is known that under terrestrial conditions, silicon is the main material in photovoltaics, but the relatively low efficiency of photocells based on monocrystalline silicon has led to the need to obtain semiconductor materials with a wide spectral sensitivity to solar radiation [1, 2].

Obtaining new semiconductor materials with heterojunctions is one of the main areas of instrument engineering and photoenergy. In this regard, well-known and widely used semiconductor structures based on heterojunctions demonstrate new features that make it possible to obtain new high-speed devices and efficient photocells with a wide spectral range. For this reason, well-known and widely used semiconductor materials with heterojunctions are always in the focus of attention of scientists and specialists. Obtaining heterojunctions and studying their electrophysical, photoelectric, optical properties is a relevant area of electronics. These studies allow creating new electronic devices or improving the parameters of existing devices for practical application in various fields of science and technology [3, 4].

At present, Scientists and specialists pay special attention to increasing the lifetime of minority charge carriers, thermal stabilization and radiation resistance of silicon due to the introduction of impurity atoms, the formation of various compounds and clusters, which leads to a change in the fundamental parameters of the original material. A physical mechanism for cluster formation has been created, and technological methods for obtaining silicon with clusters of various impurity atoms have been developed. In this direction, the possibilities of obtaining highly efficient photocells based on semiconductor materials doped with various impurity atoms have also been shown. In the environment of these materials, silicon is and remains the main material developed by planar technology and allowing to obtain a variety of electronic devices and devices without complex technological operations. However, to obtain silicon doped with various impurity atoms, it is necessary to develop a reproducible diffusion technology. Silicon doped with germanium impurity atoms is a promising material in the modern electronics industry, especially in the field of optoelectronics, which requires further detailed study of diffusion technologies for obtaining and studying the electrical, photoelectric and optical properties of these materials [5–7].

The aim of this work is to investigate the potential of the GexSi1-x quasi-heterostructure in silicon-based solar energy. This material is of particular interest because varying the parameter x allows for an expansion of silicon's spectral sensitivity into the infrared region, which is especially important given that approximately 40% of solar radiation falls within this range. Thus, this study focuses on determining the optimal parameters of Si-Ge structures to facilitate the development of highly efficient solar cells of the future.

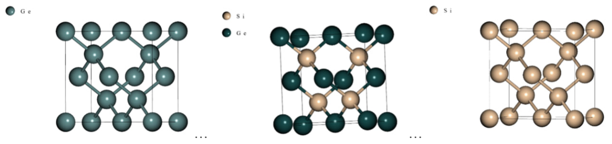


Fig. 1. Elementary lattice of silicon doped with germanium with the structure in the case of x = 1, x = 0.5, x = 0.

2. Materials and methods

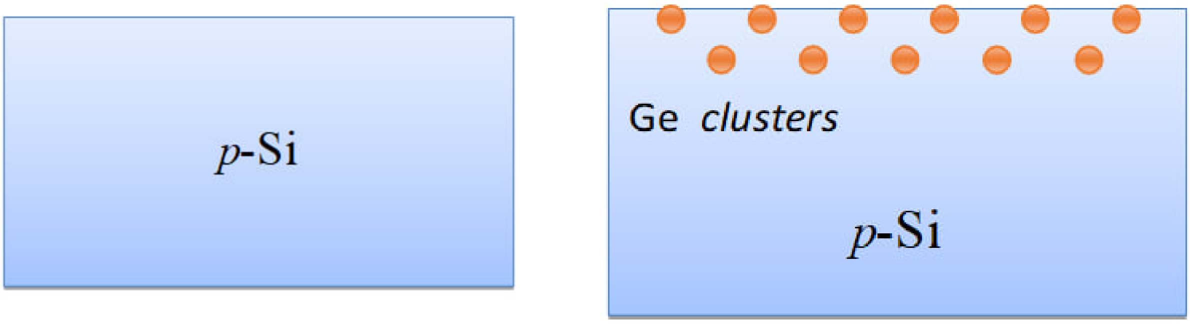
The lattice constants of silicon and germanium differ from each other, and during epitaxial growth of germanium on silicon, a lattice mismatch of the order of 4.18% appears [8]. To avoid such a mismatch, the thickness of the grown germanium on the silicon surface should not be greater than a critical value. The critical thickness of the epitaxial germanium layer is of the order of 1 nm . Therefore, it is of interest to obtain a near-surface region enriched with germanium in the silicon lattice by the diffusion method. Since the solubility of germanium in silicon is infinite [9, 10]. To obtain Ge_xSi_{1-x} structures based on silicon, we used low-temperature diffusion technologies [11, 12]. As the initial silicon, we used p-type single-crystal silicon with a resistivity of 0.5 Ohm*cm. Powdered germanium with a purity of 99.99% was used as an impurity. Silicon measuring $4 \times 8 \times 1$ mm^3 and containing 12 mg Ge impurity was placed in an evacuated quartz ampoule. The furnace temperature was gradually increased at a rate of 10 deg/min from room temperature. Then the samples were heated to the temperature of the first stage of impurity atom diffusion for germanium, which is in the range $\mathrm{T} = (900 - 950)°\mathrm{C}$. They were maintained at this temperature for $\mathrm{t} = (10 - 30)$min. Then the furnace temperature was raised fairly quickly $(150 \div 200\mathrm{deg/min})$ to a temperature of $\mathrm{T} = 1200 \div 1250°\mathrm{C}$. The samples were maintained at this temperature for $\mathrm{t} = 5 \div 20$ hours, after which the quartz ampoules were removed from the furnace and cooled at a rate of 40°C/sec.

The results of the study showed that, unlike samples obtained by the traditional method, during diffusion in samples using the new technology, no erosion is observed on the surface and silicides are not formed on the surface or in the near-surface region of silicon.

After diffusion of the near-surface region of silicon, an enriched germanium layer with a decreasing concentration distribution over depth is formed. Thus, a quasi-heterostructure Ge_xSi_{1-x} is obtained. Fig. 1 shows the change in the crystal lattice of silicon from the surface over depth (from left to right), compositions $Ge_1Si_0, \ldots, Ge_{0.5}Si_{0.5}, \ldots, Ge_0Si_1$, simulated using the program Quantum ESPRESSO.

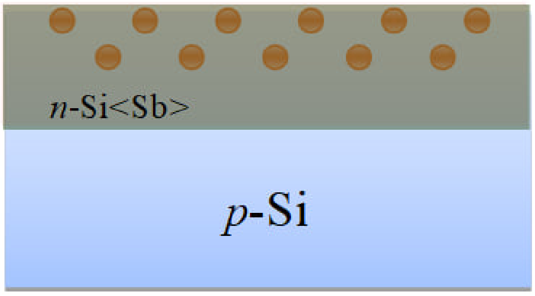
Analysis of literature data showed that all solar cells with a thin continuous layer of germanium, i.e. heterojunctions with silicon, have the same structure [13–15]. On the radiation side, a thin layer of silicon is created, then comes the epitaxial layer of germanium and then the main substrate. It is clear that the forbidden zone of silicon is 1.12 eV, and for germanium it is 0.68 eV. In this case, silicon acts as a transparent window for germanium. In our case, there is a place for the passage of radiation between the formed germanium clusters. In addition, light radiation has the ability to overcome obstacles. Therefore, it is possible to create ap - n junction near the surface of silicon, which is doped with germanium. The inverse structure has a disadvantage, firstly, the light intensity drops sharply after passing the entire substrate. Secondly, from the quasi-heterojunction to the $p - n$ junction is a long way for separating charge carriers.

$p - n$ transition was obtained with the introduction of impurity atoms of antimony in silicon of the KDB- 0.5



(a) Initial and control sample KDB-0.5.

(b) After diffusion of germanium.



(c) With $p-n$ junctions.

Fig. 2. Stages of obtaining a solar cell based on silicon with Ge_xSi_{1-x} quasi-heterojunctions.

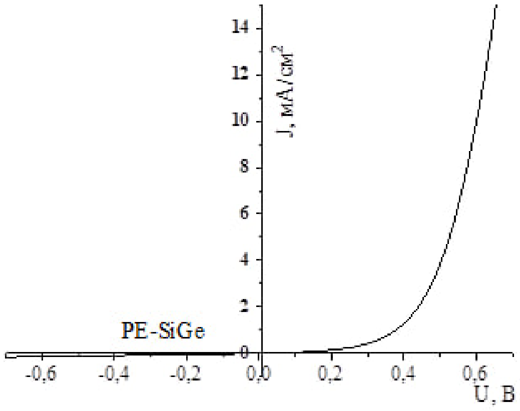


Fig. 3. Current-voltage characteristics of silicon samples doped with germanium and antimony impurity atoms.

brand, the depth of the $p-n$ junction was from 0.5 to 6μ m. The current-collecting contacts of the solar cells were manufactured by thermal evaporation of nickel in a vacuum (VUP-5 units). A layer of SiO_2 with a thickness of $\sim$ 1000 was used as a light-antireflective coating. The photocells were made in the form of a parallelepiped measuring 2×2 cm^2. Fig. 2 shows the design of the obtained photocells based on silicon with $Ge_xSi_{1-x} - Si$ quasi-heterostructures.

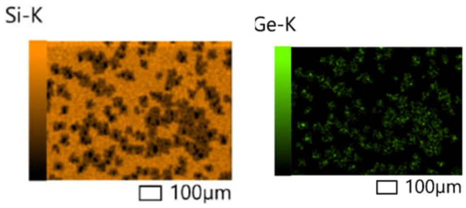


Fig. 4. Surface topography of a silicon sample after doping with germanium impurity atoms.

After doping with germanium, a $p-n$ junction was formed. As an impurity to obtain an -layer, we used Sb atoms . The choice of impurity was based on the properties of germanium, that in the volume of clusters enriched with germanium, also obtain an n-type. Fig. 3 shows the current-voltage characteristics of the obtained $p-n$ structures. transition from Ge_xSi_{1-x}, measured on a Keithley 2450 setup.

After obtaining silicon doped with germanium, the surfaces were examined using SEM (JSM-IT 200 SEM). Energy dispersive analysis shows that a germanium cluster in the form of islands does indeed appear on the silicon surface.

The results of the experiments showed that it is impossible to obtain a thin layer of germanium on the silicon

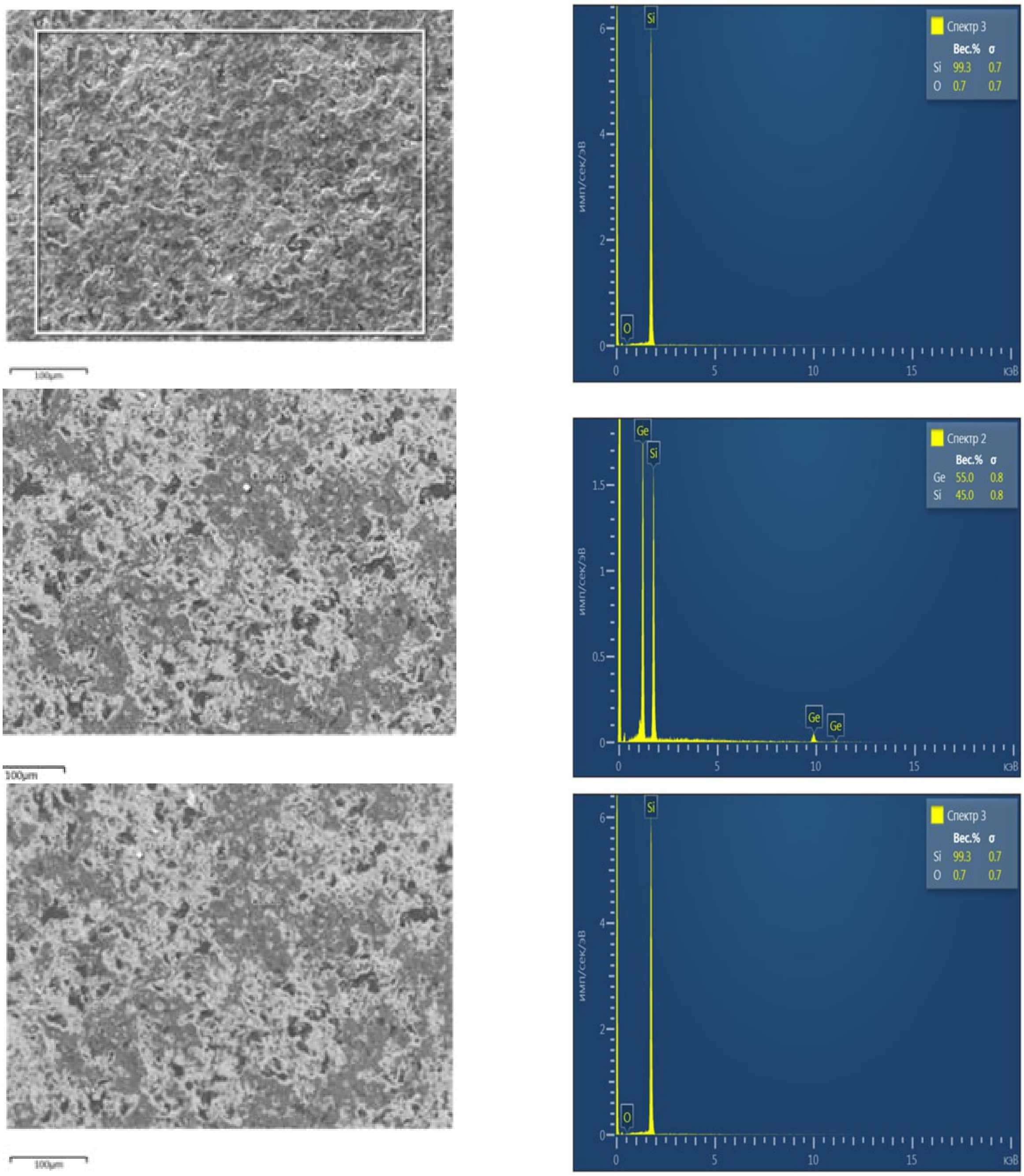


Fig. 5. *a* – surface topography of a silicon sample after doping with germanium, *b* – results of X-ray energy dispersive microanalysis.

surface by the diffusion method, as well as by the epitaxial method. During the diffusion process, germanium impurities on the silicon surface are collected in many small circles and diffuse further. As a result, micro- and nano-sized clusters are obtained in the form of islands on the near-surface region of silicon (Fig. 4). Such a structure requires a new approach for its use in solar cells. It can be assumed that each cluster is a quasi-heterostructure in the form of Ge_xSi_{1-x} along the depth of silicon.

3. Results and discussions

The surfaces of the obtained samples were independently examined using another electron microscope. Fig. 5 shows the topography of the front side of the sample, obtained using a scanning electron microscope (Mira Tescan 3).

Elemental analysis of the sample surface showed that

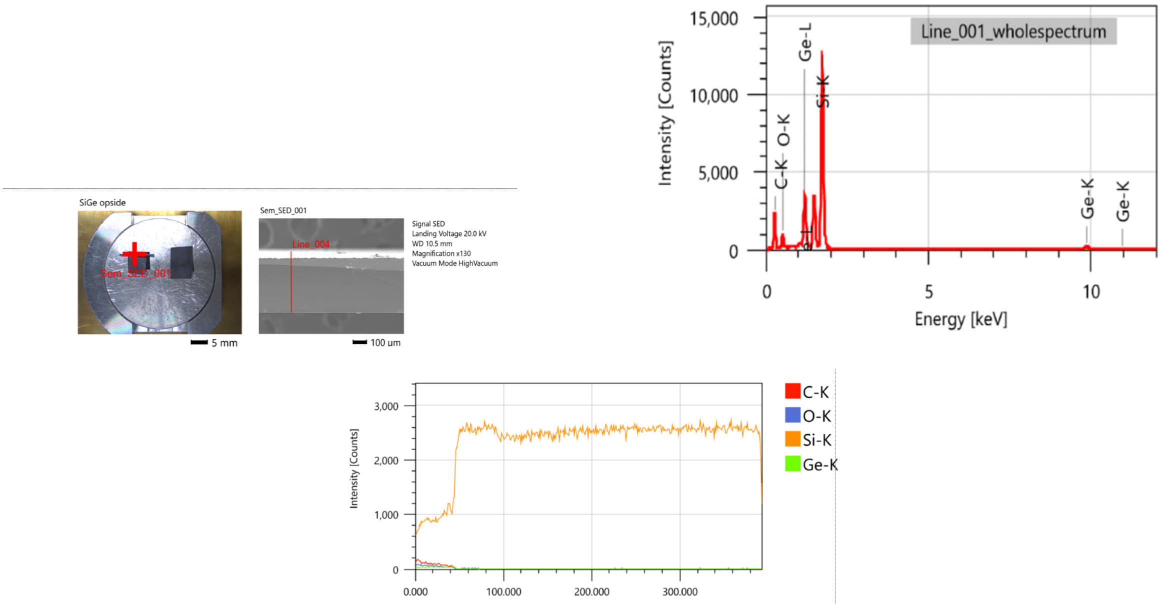


Fig. 6. Micrograph of the side face of silicon samples with impurity atoms of germanium after diffusion and energy-dispersive X-ray microanalysis of the side face of silicon samples doped with impurity atoms of germanium obtained by the EDX method.

the concentration of silicon (in atomic percent) was ∼ 64.46%, germanium ∼ 26.9%, oxygen 5.93%, and other elements 2.71%. It was assumed that germanium clusters with a composition of approximately $Ge_{27}Si_{73}$ were formed on the silicon surface and in the front part.

Fig. 6 shows a micrograph of the end side (side) of a silicon sample with a $Ge_xSi_{1-x} - Si$ heterostructure, obtained using SEM. From the analysis of the obtained results it was established that with the depth of the silicon sample the concentration of carbon and oxygen decreases, and the concentration of silicon atoms increases. As can be seen from Fig. 6, impurity germanium atoms are present on the surface and near the surface of silicon to a depth of 6-8 μm.

A comparative analysis of the diffraction pattern of silicon doped with impurity atoms of germanium for the elements Si, Ge and SiGe obtained from the open crystallographic database COD (Crystallography Open Database) is presented. The spectrogram of X-rays reflected from the surface of a sample of silicon doped with impurity atoms of germanium formed several main peaks. The lines corresponding to International open database of crystallographic materials Ge and Si were superimposed to identify the resulting peaks [16–18].

Using the data obtained from X-ray analysis, it can be calculated that the peaks (25.39; 27.25; 28.35; 29.85; 35.25; 37.2; 37.8; 54.1; 68.4; 69.41; 76.55) form Ge_xSi_{1-x} compounds on the surface of Si. Based on the literature review and what we have learned from the international (Crystallography Open Database) it was determined that the peaks for Si 28.35; 37.8; 69.41; 76.55 corresponding to the crystallographic planes [131], [040], [313] in the general spectrum of the diffraction pattern (Fig. 7). It was found that the peaks 27.25; 46.2; 54.1; 68.4 correspond to germanium atoms. Analysis of the results of the study showed that the identified four peaks do not belong to Ge or Si atoms, and two of them (25.39; 46.2) are estimated to belong to silicon with $Ge_xSi_{1-x} - Si$ heterostructures. It is known that the lattice constants of Ge and Si are a = 5.63 and a = 5.34, respectively. The lattice constant (a) and the diffraction lattice constant $(\mathrm{d_{hkl}})_{\mathrm{o}}$ f the binary compound of Si and SiGe formed on its surface were calculated using X-ray structural analysis data using the following Eqs. (1) and (2).

$$a = d_{hkl} \cdot \sqrt{h^2 + k^2 + l^2} \tag{1}$$

$$d_{hkl} = \frac{\lambda}{2 \cdot \sin\theta} \tag{2}$$

where θ is the Bragg angle and $\lambda = 0.15402$ nm (wavelength).

The results of the study of the photoelectric properties of silicon samples doped with germanium atoms showed that the spectral sensitivity of these samples expands in the infrared region. Fig. 8 shows the spectral dependence of the short-circuit current of the obtained $p - n$ junction structures based on silicon doped with germanium atoms (curve 1) and after thermal annealing at a temperature of $T_{dg} = 850°C$ (curve 2). Measurements were carried out in

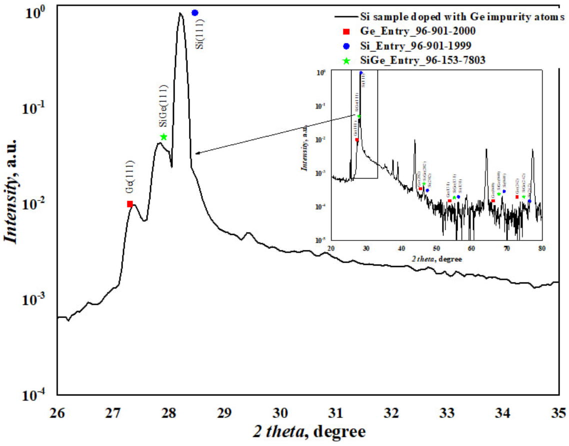


Fig. 7. Diffraction pattern of silicon doped with germanium impurity atoms.

an IKS-12 spectrometer ($\lambda = 0.496 \div 3.872\mu$ m) at a radiation power density of $P = 510^{-6}$ W/cm^2. It was found that the spectral dependence of the short-circuit current in Ge$_x$Si$_{1-x}$ structures formed in the silicon crystal lattice differs significantly from the short-circuit current values in those subjected to additional thermal annealing, i.e. the photosensitivity of the samples shifted from the visible to the infrared. The obtained results can be explained by the absorption of incident photons by germanium atoms in the studied spectral region.

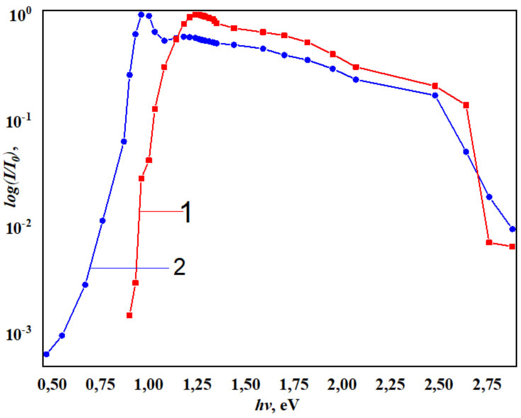


Fig. 8. Spectral dependence of the short-circuit current of silicon samples with a $p - n$ junction 1 - SiGe after diffusion $T_D = 1200°C$, 2 – SiGe after thermal annealing at a temperature $T_{OD} = 850°C$.

It is noted that germanium doping can lead to the formation of denser small-sized voids, which can be easily eliminated by high-temperature annealing, and can improve the integrity of the gate oxide of semiconductor devices. Meanwhile, the oxygen gettering ability in silicon can be enhanced by germanium, so that the intrinsic gettering ability of the wafers is improved. In addition, it has been reported that germanium can suppress the formation of thermal donors [19–23].

Table 1. Solar cell parameters.

P.V.	Si Sb	Si /SiGe
After diffusion of antimony with Tdiff = 1200°C		
J_{shc} , mA/cm^2	16.2	17.6
U_{xx}, mV	384	426
Post maintenance T_{TO} = 850°C		
J_{shc} , mA/cm^2	18.9	19.3
U_{xx}, mV	412	423

After diffusion, a sunlight simulator based on an incandescent lamp with corrective filters was used to perform measurements under the same conditions. Table 1 shows the parameters of the solar cell without germanium atoms, the parameters of the solar cell with germanium clusters, and the parameters of the solar cell with germanium clusters after treatment at 850 °C for 3 hours to increase the formation of microjunctions. SiGe in the silicon crystal lattice.

4. Conclusions

Thus, on the basis of silicon doped with impurity atoms of germanium, it is possible to create heterojunctions that expand the range of spectral photosensitivity and increase the efficiency of the created solar cells. It has been established that the formation of Ge$_x$Si$_{1-x}$ compounds in silicon leads to a change in the band gap width of the original material. It has been shown that the change in the band gap width of the initial silicon due to the formation of binary Ge$_x$Si$_{1-x}$ compounds alters one of the fundamental parameters of the material, which, in turn, leads to an expansion of the spectral sensitivity range. This is characteristic when developing efficient photovoltaic cells with a wide range of solar radiation absorption.

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