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Diffusion-Driven Formation Processes Structural Characteristics and Optica l–Parametric Properties of GexSi1–x Alloys

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Diffusion-Driven Formation Processes, Structural Characteristics, and Optical–Parametric Properties of Ge_xSi_{1-x} Alloys

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Abstract. In this study, a two-stage diffusion method was developed and applied to introduce germanium atoms into monocrystalline silicon and form nanoscale silicon–germanium (Ge_xSi_{1-x}) compound layers. Due to the extremely low diffusion coefficient of Ge in silicon, direct incorporation of germanium atoms into the silicon lattice is technologically challenging. By gradually increasing the temperature during the diffusion process, controlled Ge_xSi_{1-x} layers with well-defined composition and thickness were successfully synthesized. Structural and compositional analyses conducted using FTIR and SEM confirmed the formation of Si–Ge clusters with a size of 1–2 µm and high surface density. According to EDX microanalysis, the near-surface layer consisted of approximately 44% Si, 38% Ge, and 15% O, indicating that nearly half of the elemental composition was germanium. Optical measurements performed using a SHIMADZU UV-2700i spectrophotometer revealed that the bandgap energy of the synthesized Ge_xSi_{1-x} compounds ranged from 0.75 to 1.12 eV. As the silicon content in the compound increased to around 60–65%, the bandgap value approached that of monocrystalline silicon (E_g = 1.12 eV) and remained stable. FTIR spectra also demonstrated the presence of GexSi1 -x compounds through the characteristic absorption peak at 1066 cm^{-1}. The obtained results show that the proposed diffusion technique enables the fabrication of stable Ge_xSi_{1-x} layers suitable for high-efficiency heterostructure solar cells, optoelectronic detectors, and simple electronic devices that do not require complex fabrication processes. The promising optoelectronic and structural properties of these materials make them strong candidates for next-generation nanoelectronic and photonic applications.

INTRODUCTION

The development and large-scale implementation of modern electronic devices based on semiconductor materials is considered one of the most promising directions for attracting foreign investment and strengthening technological competitiveness. In Uzbekistan, sustainable progress in the field of electronics is directly linked to the renewal of existing industrial infrastructure, modernization of production facilities, and the integration of advanced technologies into manufacturing processes. Therefore, continuous upgrading of equipment, improving technological efficiency, and aligning production lines with global market requirements are essential tasks for enterprises operating in the electronic industry.

The fabrication of semiconductor-based electronic components involves multistage technological processes that require high precision, strict control, and the coordinated application of complex physical and chemical procedures. Among such materials, silicon–germanium (Ge_xSi_{1-x}) alloys have become highly significant in monocrystalline silicon electronics and especially in nanoelectronics. Due to their advantageous electrophysical characteristics, these alloys are widely utilized in high-frequency devices, sensors, integrated circuits, and high-efficiency micro- and optoelectronic components [1–8]. Furthermore, Ge_xSi_{1-x} alloys demonstrate several advantages over traditional A_3B_5 and A_2B_6 semiconductor materials, including greater resistance to external influences, enhanced thermal stability, and favorable band-structure properties that make them suitable for next-generation electronic device fabrication.

Traditionally, Ge_xSi_{1-x} alloys are synthesized through liquid-phase epitaxy or vapor-phase deposition techniques, where Ge and Si atoms chemically bond to form epitaxial layers [8–12]. However, these approaches are limited in their ability to accurately control layer thickness, compositional gradients, and atomic-scale uniformity. They also present challenges in forming stable nanoscale Ge–Si structures within the silicon crystalline lattice.

Recent studies have shown that by gradually modifying the diffusion temperature, controlling the diffusion rate, and optimizing the sequence of technological stages, it is possible to obtain Ge_xSi_{1-x} binary layers with precisely controlled composition and thickness directly within a silicon monocrystal [13-15]. This approach enables fine-tuning of diffusion kinetics, compositional uniformity, and lattice incorporation, thereby facilitating the formation of highly effective nanoscale Ge_xSi_{1-x} structures suited for advanced electronic applications [16-18].

EXPERIMENTAL RESEARCH

The diffusion of germanium impurity atoms into monocrystalline silicon is considered technologically and economically challenging due to the extremely low diffusion coefficient of Ge atoms in silicon. By employing a newly developed two-stage diffusion method, Ge_xSi_{1-x} alloy cells were successfully formed on the surface and near-surface region of silicon, enabling the creation of a heterostructure at the transition boundary between the alloyed layer and the monocrystalline silicon substrate [19-22].

Analysis of scientific literature shows that the temperature dependence of the diffusion coefficient of germanium impurity atoms in silicon is calculated using the following expression:

$$\mathrm{D} = 6 \cdot 10^5 \exp\left(-\frac{5{,}28}{\mathrm{kT}}\right) \tag{1}$$

Based on this equation, the diffusion coefficient of Ge atoms in silicon at T = 1250 °C is theoretically estimated to be extremely small, approximately

$$\mathrm{D} \sim 4 \cdot 10^{-13}\ \mathrm{sm}^2/\mathrm{V} \cdot \mathrm{s}$$

In the experiment, the diffusion of germanium impurity atoms into silicon was carried out by gradually increasing the temperature and smoothly reaching the required diffusion point. For this purpose, the MAGNETIC-type vacuum tube electric furnace was heated from room temperature to T = 950 °C over a period of t = 2 hours, and the silicon samples were held at this temperature for t = 30–40 minutes. After this pre-diffusion stage, the samples underwent the main diffusion process at T = 1250 °C for t = 10 hours.

The experiment was repeated several times, and during each cycle three silicon samples were placed inside a quartz ampoule. As a result of the diffusion, the silicon structure shown in Figure 1 was obtained.

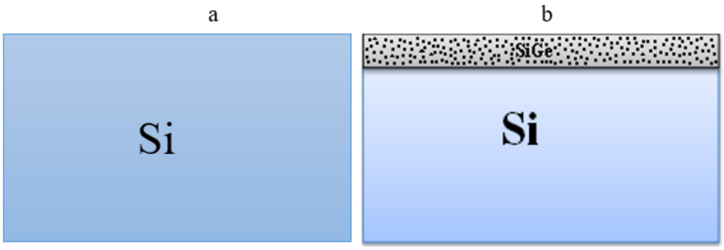

Figure 1.(a) Initial silicon sample of the KEF-100 grade; (b) distribution of germanium atoms introduced into silicon by the diffusion method.

To verify the formation of the structure depicted in Figure 1, the surfaces of silicon samples implanted with germanium atoms after the diffusion process were analyzed using a FTIR microscope (Figure 2) and a scanning electron microscope (SEM, Figure 3). The analysis indicated that the silicon-germanium compound clusters formed on the surface measured approximately 1–2 µm in size, with a high density of such clusters observed across the sample surface (Figure 2a). Following the removal of the surface layer, about 5–6 µm thick, through mechanical polishing (lapping), subsequent FTIR examination of the polished silicon surface revealed a substantially reduced presence of Ge_xSi_{1-x} type binary compounds (Figure 2b).

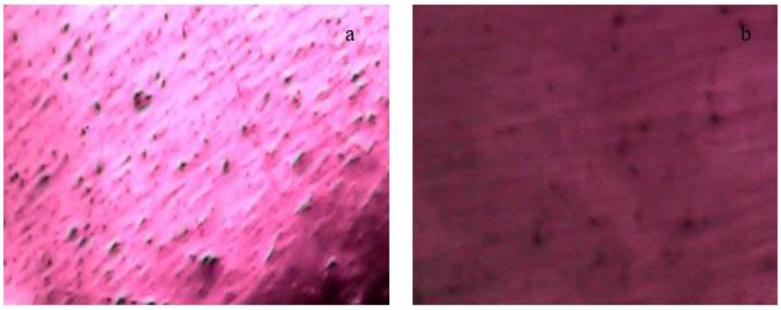

Figure 2. a) Appearance of Ge_xSi_{1-x} compounds formed in monocrystalline silicon after germanium atom diffusion. b) Surface of silicon after removal of a 5–6 µm layer by polishing.

Figure 3 shows the surface topology of a silicon sample containing Ge_xSi_{1-x} compounds, obtained using a JSM-IT 200 scanning electron microscope (SEM). The compositional distribution of the layer containing germanium atoms on the silicon surface is presented in Figure 3b.

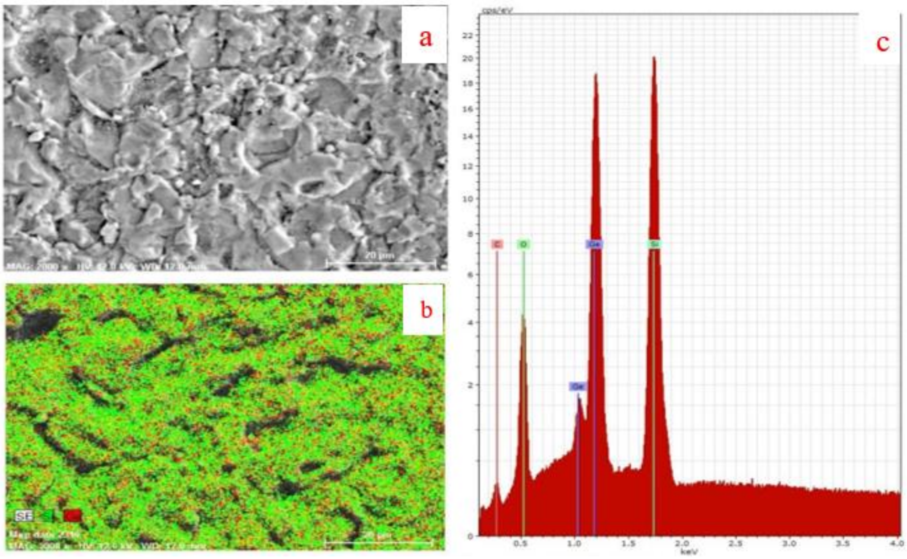

Figure 3. a and b – Topology of silicon doped with germanium atoms, c – Results of energy-dispersive X-ray microanalysis (EDX) (scale: 20 µm).

Table 1. Elemental composition of the sample based on SEM-EDS analysis (wt.%)

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**	

The results of the study indicate that after germanium atoms were diffused into the silicon surface, a thin compound layer was formed, with the elemental composition of this layer expressed in percentages (Figure 3c).

Based on energy-dispersive X-ray (EDX) microanalysis, the concentrations of atoms in the silicon surface and near-surface region were determined as follows: silicon ~44.32%, germanium ~38.11%, oxygen ~15.58%, and carbon ~1.98%. These findings demonstrate that in the near-surface layer of the silicon crystal, the amount of germanium atoms accounts for nearly half of the total elemental composition

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The bandgap energy of Ge_xSi_{1-x} compound cells formed on the surface of monocrystalline silicon was measured using an optical method with a SHIMADZU UV-2700i spectrophotometer, while preserving the Ge_xSi_{1-x} compound layer on the silicon surface. In the experiments, the measured bandgap of the Ge_xSi_{1-x} compounds ranged from Eg = 0.75 to 0.8 eV, which is higher than the bandgap of pure semiconductor germanium. Figure 4 shows the relationship between the bandgap energy of the silicon-germanium compounds and the composition of the GexSi1-x binary compounds formed on the silicon surface.

Analysis of the physical mechanism of the formed compounds indicated that as the silicon content in the compound increased up to 65%, the bandgap energy of the resulting compound rose from 0.75 eV to 1.12 eV, reaching the bandgap energy of silicon. When the silicon content in the compound exceeded approximately 60%, the bandgap energy remained nearly unchanged, corresponding to the fundamental bandgap of monocrystalline silicon (Eg = 1.12 eV). These findings were confirmed through experiments conducted on multiple silicon samples with germanium atom diffusion.

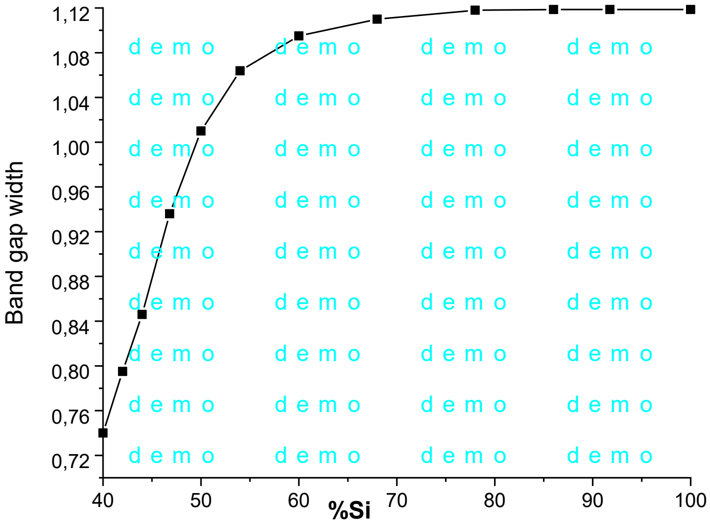

Figure 4. Dependence of the bandgap of silicon-germanium compounds on the elemental composition of the formed compound.

The composition and optical properties of the obtained Ge_xSi_{1-x} compounds were investigated using a Fourier-transform infrared (FTIR) spectrometer, FSM-1202. Before studying the optical properties of the silicon samples obtained after diffusion, both surfaces of the samples were polished using a polishing device with diamond paste, and the remaining four edges of the samples were removed to a depth of approximately 100 µm. This preparation allowed for precise measurement of the composition of the resulting Ge_xSi_{1-x} compounds. The measurement results are presented in Figure 5, and their analysis led to the following conclusions.

The FTIR spectrum presented in Figure 5 clearly illustrates the optical response of the Ge_xSi_{1-x} compounds formed in monocrystalline silicon as a result of germanium diffusion. The absorption features observed near 850–885 cm^{-1} correspond to the vibrational modes of Ge–O_2 and Ge–O–Si bonds, indicating partial oxidation of germanium during the diffusion process. Distinct peaks in the 995–1008 cm^{-1} region are attributed to stretching vibrations of Si–O–Ge linkages, confirming the formation of mixed silicon–germanium oxide structures. The pronounced absorption band at 1066 cm⁻¹ represents a characteristic vibrational mode of the Ge_xSi_{1-x} alloy, demonstrating that germanium atoms were successfully incorporated into the silicon lattice. The feature detected around 1104 cm⁻¹ is associated with Ge–O vibrational modes, suggesting the presence of a thin germanium oxide layer at the sample surface. The consistent distribution of these peaks across the spectrum reflects the simultaneous formation of several types of chemical bonds within the surface and near-surface regions of silicon. The relatively high intensity of the Ge_xSi_{1-x} absorption mode indicates a significant concentration of germanium within the modified silicon layer.

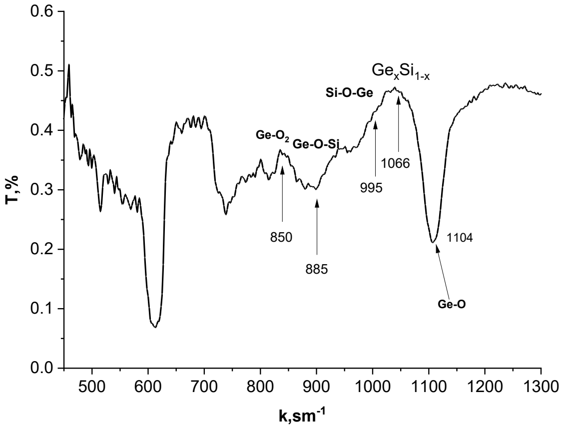

Figure 5. IR absorption spectrum of silicon samples containing Ge_xSi_{1-x} compounds.

These FTIR observations are in agreement with SEM and EDX analyses, both of which confirm the formation of an ultrathin Ge_xSi_{1-x} compound layer on the silicon surface. Such spectral characteristics demonstrate that the diffusion process enabled stable formation of silicon-germanium structures with well-defined chemical composition. Overall, the FTIR analysis verifies that the resulting Ge_xSi_{1-x} layers exhibit physical–chemical properties suitable for various optoelectronic applications.These findings are also supported by conclusions reported by other authors [23-25].

CONCLUSIONS

In this research, a two-stage diffusion technique was successfully developed to incorporate germanium atoms into monocrystalline silicon, enabling the formation of nanoscale Ge_xSi_{1-x} layers with precisely controlled composition and thickness. Structural and compositional analyses using SEM, FTIR, and EDX confirmed the presence of densely packed Si–Ge clusters, with germanium comprising nearly half of the near-surface elemental composition [26-36]. Optical measurements revealed that the bandgap of the synthesized compounds ranged from 0.75 to 1.12 eV, approaching the bandgap of pure silicon as the silicon content increased to approximately 60–65%. FTIR spectra further validated the formation of stable Ge_xSi_{1-x} compounds, indicated by characteristic absorption features. These results demonstrate that the proposed diffusion method enables the fabrication of robust Ge_xSi_{1-x} layers suitable for high-efficiency heterostructure solar cells, optoelectronic detectors, and simple electronic devices, highlighting their potential for next-generation nanoelectronic and photonic applications.

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