



REGULAR ARTICLE

X-Ray and Raman Spectroscopy of $(\text{Si}_2)_{1-x}(\text{BP})_x$ Binary Compounds in Silicon

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(Received 07 August 2025; revised manuscript received 18 October 2025; published online 30 October 2025)

This study investigates the interaction of phosphorus and boron impurity atoms in silicon using X-ray and Raman spectroscopy. Two groups of samples were prepared: the first group was doped with phosphorus atoms first, followed by boron atoms; in the second group, boron atoms were introduced first, followed by phosphorus atoms. Raman spectroscopy was used to analyze the formation of binary compounds of phosphorus and boron atoms in the silicon matrix, as well as their optical, photoelectric, and structural properties. The results showed that when phosphorus and boron atoms are present together in silicon, they significantly alter the crystal structure and electrical conductivity properties. Samples doped with phosphorus exhibited higher electrical conductivity and photoelectric properties, while samples doped with boron showed lower optical and electrical properties. The data obtained from Raman spectroscopy clearly demonstrated the atomic interactions and crystal structure. Additionally, the microstructural properties of the samples were studied using SEM (Scanning Electron Microscopy) and AFM (Atomic Force Microscopy). SEM analysis revealed the uneven distribution of boron and phosphorus atoms and nano-scale structures, while AFM analysis identified fine changes and structural defects on the surface of the doped silicon materials. The results of this study expand the possibilities for controlling the properties of semiconductors by doping silicon with impurity atoms and forming binary compounds, contributing to the development of new technological solutions and materials, especially in optoelectronics and sensor technologies.

Keywords: Semiconductor, Silicon, Boron, Phosphorus, Raman Spectrum, Scattering, Spectrometer, Laser, Diffusion.

DOI: [10.21272/jnep.17\(5\).05009](https://doi.org/10.21272/jnep.17(5).05009)

PACS numbers: 61.05.cp, 61.82.Fk, 73.43.Qt

1. INTRODUCTION

As is known, elements of groups III and V in silicon are mainly located in the sublattice sites and create shallow donor and acceptor energy levels in the band gap of silicon. The solubility of these elements in silicon is quite high and reaches $N = 10^{21} \text{ cm}^{-3}$. In the atomic state, they are in the form of singly charged $\text{A}^{\text{III-}}$, $\text{B}^{\text{V+}}$ ions and create an electric potential around themselves, they also create a corresponding additional concentration of charge carriers both in the conduction band and in the valence band. All this leads to a significant violation of the thermodynamically equilibrium state of the crystal. Therefore, the crystal under such conditions is in a thermodynamically nonequilibrium state [1-3].

A high concentration of phosphorus during diffusion from the deposited silicon surface layer is presented in the literature [4]. At the highest area concentration to the surface, diffusion is controlled through doubly negative vacancies, and this change in diffusion mechanisms leads to the characteristic kink and tail

profiles commonly observed in phosphorus scattered emitters of Si solar cells.

In this work, we studied the optical properties of silicon samples doped with impurity atoms of phosphorus and boron.

2. METHODOLOGY

Single-crystal silicon grade ($N_{\text{P}} \sim 4 \cdot 10^{15} \text{ cm}^{-3}$) with oxygen content $N_{\text{O}_2} \approx (5 \div 6) \cdot 10^{17} \text{ cm}^{-3}$ and dislocation density $N_{\text{D}} \sim 10^3 \text{ cm}^{-2}$ [5, 6]. The size of the samples was $V \sim 0.38 \times 4 \times 6 \text{ mm}^3$.

Two types of samples were chosen for the study. The first group of samples consisted of initial silicon. The second group of samples consisted of silicon, first doped with impurity phosphorus atoms and then with impurity boron atoms.

The diffusion of phosphorus was carried out from the deposited layer of ammonium phosphate at $T = 1100^\circ\text{C}$ for $t = 2$ hours in the open air. Boron diffusion was also carried out at a temperature of $T = 1100^\circ\text{C}$ for $t = 2$ hours in the open air, using a boron nitride plate as a source, located

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horizontally above the sample at a distance of 0.4 mm. This choice of diffusion conditions in silicon was determined by the requirement to obtain the maximum concentration of boron atoms.

After diffusion, phosphorosilicate and borosilicate glass was removed from the surface by etching in HF acid. The surface concentration of impurity atoms of boron and phosphorus in silicon was measured by the 4-probe method.

Raman spectroscopy is an effective method for

chemical analysis and composition studies. Raman spectroscopy is very sensitive to inorganic elements and clusters of silicon crystal lattices [7-8].

The Raman spectra were measured using a Raman spectrometer (Spectrometer manufactured by Horiba (MacroRAM, Affordable Benchtop Raman Spectrometer)). The measurement area is from 100 cm^{-1} to 3400 cm^{-1} . Approvals make 785 nm diode lasers the industry standard.

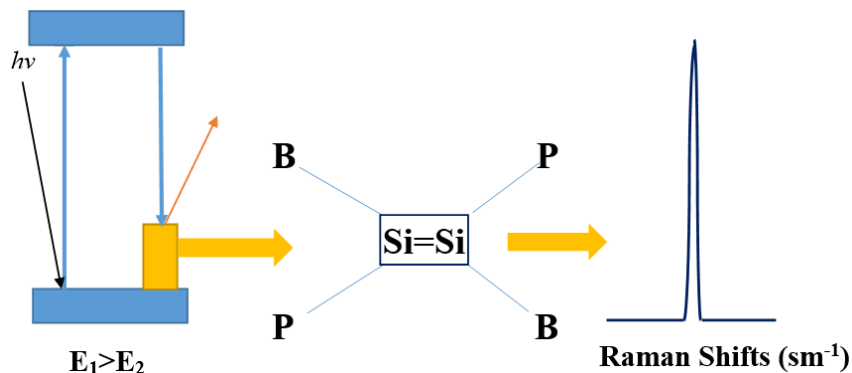


Fig. 1 – Model of the Raman spectrum of impurity atoms of phosphorus and boron in silicon

Samples of the second group had *p*-type conductivity on the surface, the surface concentration of boron was about $N_B \approx 4 \cdot 10^{19}\text{ cm}^{-3}$. The samples of the third group had *n*-type conductivity, the surface concentration of phosphorus was about $N_P \approx 3 \cdot 10^{20}\text{ cm}^{-3}$.

The elemental composition of silicon samples doped with boron and phosphorus impurity atoms was studied on a MacroRAM Raman spectrometer (Affordable Benchtop Raman). The spectrum measurement range of this spectrometer is from 100 cm^{-1} to 3400 cm^{-1} ; a semiconductor laser with a standard wavelength of $\lambda = 785\text{ nm}$ was used in the studies.

It is known that Raman spectroscopy is an effective method for studying the states of bonding and symmetry of interlayer atoms in semiconductors, re-cording vibrations of atoms and molecules in a crystal structure. Raman spectroscopy is also widely used to test and analyze the bond states of compounds formed by various impurity atoms in silicon [8-10].

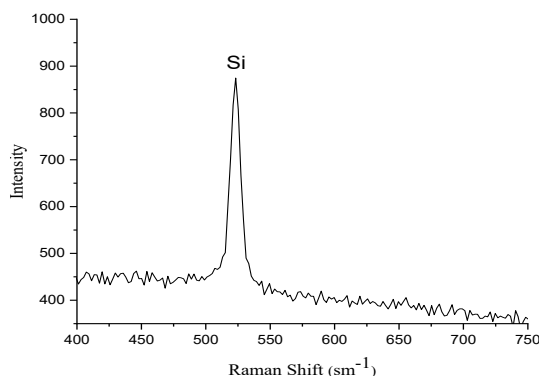


Fig. 2 – Raman spectrum of initial silicon

When obtaining the Raman spectrum of primary silicon, a peak at about 520 cm^{-1} was observed; this peak is known from the literature related to pure silicon [11-13].

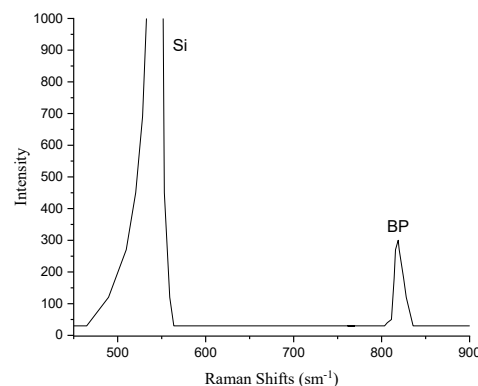


Fig. 3 – Raman spectrum of a silicon sample doped first with impurity phosphorus atoms and then with impurity boron atoms (second group of samples)

The results of comparison with the values of the Raman spectrum of the original silicon and the silicon sample doped with impurity atoms of boron and phosphorus are shown in Fig. 3. The Raman spectrum of boron and phosphorus compounds in doped silicon differed by one phonon mode peak. For group 2 samples, a Raman peak was observed at 828 cm^{-1} for the determination of boron and phosphorus (BP) compounds.

The Raman spectra measured for these samples showed the formation of a peak near the wavelength of 828 cm^{-1} for boron and phosphorus compounds. An

analysis of the experimental results revealed the formation of binary compounds of boron and phosphorus atoms in the silicon lattice separately.

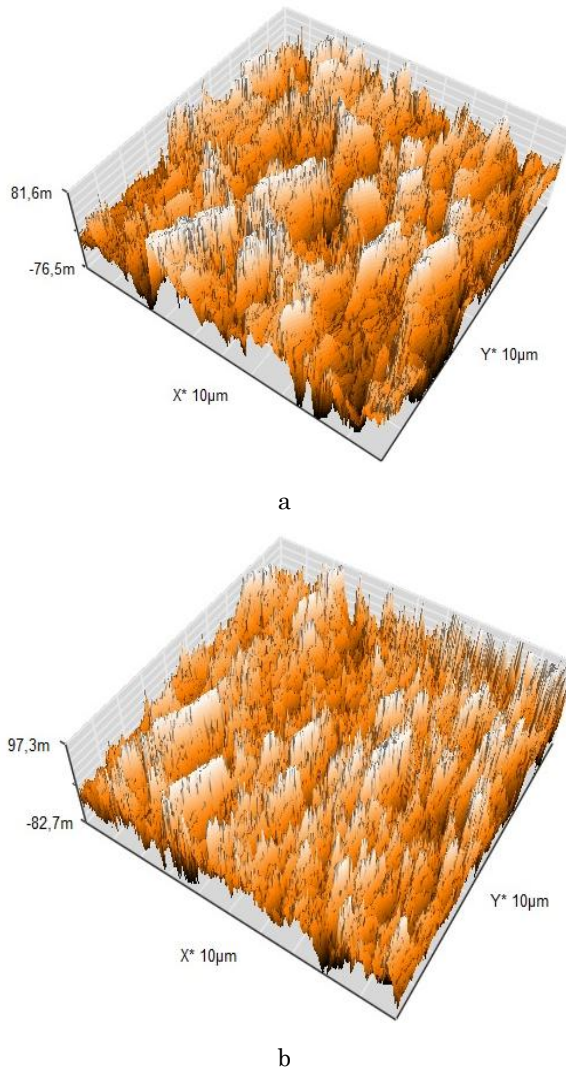


Fig. 4 – AFM images: a) initial silicon, b) silicon surface doped with impurity phosphorus and boron atoms

It is known that atomic force microscopy allows displaying the scale of a surface sample up to $\sim 10^8$ times. The device has several modes of operation. The static force mode in AFM was used for imaging in our studies. On Fig. 4 shows the surface morphology of silicon obtained by AFM. As can be seen from Fig. 4, the surface roughness of the original silicon was ~ 79.05 nm (a), and the surface roughness of silicon sequentially doped with phosphorus and boron atoms was ~ 90 nm (b).

To determine the morphology and elemental composition of the film formed after diffusion on the silicon surface, a JSM-IT200 scanning electron microscope (SEM) equipped with energy-dispersive X-ray spectroscopy (EDS) was used.

X-ray diffraction measurements were carried out using an XRD-6100 diffractometer manufactured by Shimadzu. The scanning angle range was $\theta = 20^\circ - 100^\circ$, with a scanning

speed of $2^\circ/\text{min}$ and a step size of 0.05° . The obtained data were processed using the Match! demo software.

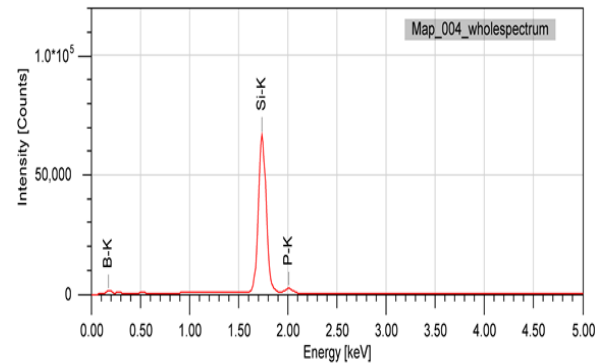


Fig. 5 – The results of the X-ray energy-dispersive microanalysis were obtained using the JSM-IT200 scanning electron microscope

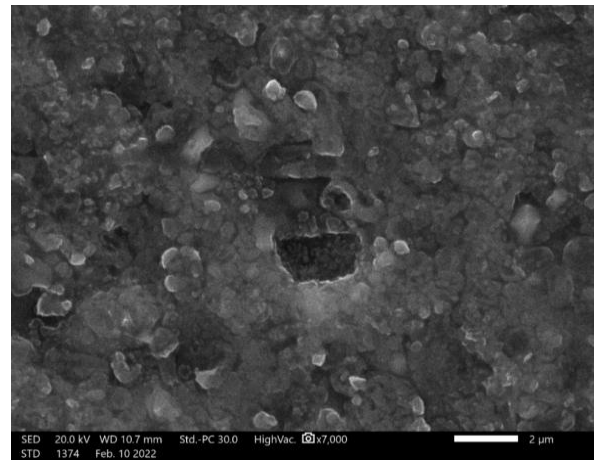


Fig. 6 – Surface morphology of the silicon sample sequentially doped with phosphorus and boron impurity atoms

The scanning electron microscopy (SEM) images distinctly reveal the surface morphological features of the synthesized $(\text{BP})_x\text{Si}_{1-x}$ -type elementary structural units. Both the high-resolution SEM micrographs and the corresponding energy-dispersive X-ray spectroscopy (EDS) data confirm the formation and compositional uniformity of the $(\text{BP})_x\text{Si}_{1-x}$ doped silicon layers. These results are presented in Figs. 5 and 6.

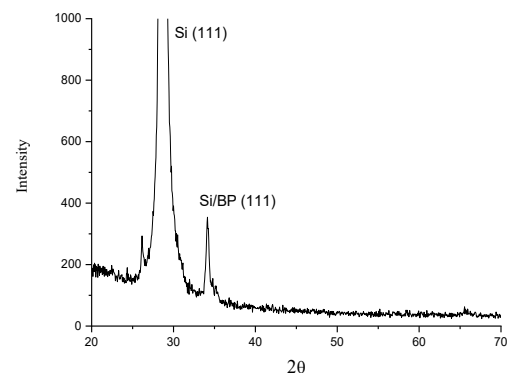


Fig. 7 – Diffraction pattern of silicon containing compounds of phosphorus and boron atoms

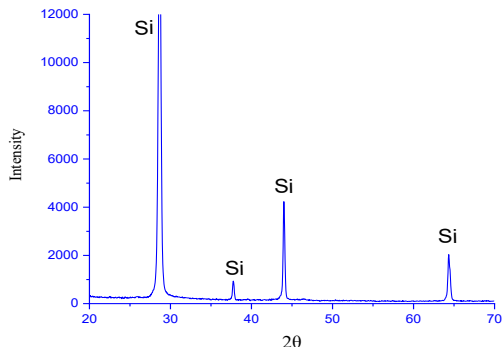


Fig. 8 – X-ray diffraction pattern of the original silicon

On Fig. 7 shows the X-ray diffraction pattern of the initial silicon. As can be seen from Fig. 7, Fig. 8 several diffraction peaks of different intensity of the incident light were observed on the diffraction pattern. X-ray peaks are observed in the initial silicon $2\theta = 28.55^\circ; 37.8^\circ; 44^\circ; 64.35^\circ$ corresponded to the basic silicon atoms in the crystal lattice. On Fig. 7 shown are the X-ray peaks of the second group of samples with peaks at $2\theta = 28.55^\circ; 34.3^\circ; 34.6^\circ; 34.75^\circ$. When comparing the diffractograms (Fig. 7 and Fig. 8), it was found that they have certain differences. New peaks observed in silicon samples doped with boron and phosphorus impurity atoms differed as follows: $2\theta = 34.3^\circ; 34.6^\circ; 34.75^\circ$. It has been established that the emerging diffraction peaks are associated with the formation of binary boron-phosphorus compounds in silicon. As can be seen from Fig. 8, in addition to the diffraction peaks corresponding to the direction of the [111]

axis of the silicon crystal, in the plane of the crystal at an angle of 34.1° . At an angle of $2\theta = 34.1^\circ$, a new diffraction peak was formed as a result of the fusion of boron and phosphorus atoms in the crystalline direction [111] [14-20].

Based on the results obtained, the lattice constants of boron and phosphorus compounds formed in silicon are calculated. The lattice constant of the resulting compound according to the Bragg law was calculated as $a = 0.4538$ nm, which corresponds to the fundamental lattice constant of the binary compound of boron and phosphorus atoms.

3. CONCLUSION

From the analysis of the spectra of the resulting Raman spectrometer, it can be said that the intensity of the peaks in the original silicon is much higher than in diffusion samples due to the formation of Si-Si bonds and bonds of the Si-B, Si-P, B-B, P-P, B-P type. It can be assumed that a binary unit cell of the $(\text{Si}_2)_{1-x}(\text{BP})_x$ type is formed in silicon doped with boron and phosphorus atoms.

X-ray diffraction analysis of the samples obtained showed the formation in silicon of compounds consisting of impurity atoms of phosphorus and boron. X-ray analysis of silicon samples doped with phosphorus and boron atoms in Figs. 7 and 8 confirmed the presence of binary boron-phosphorus compounds (B-P). It has been established that compounds of phosphorus and boron atoms are formed not during heat treatment after diffusion, but in the diffusion process itself, which was explained by the diffusion migration of phosphorus atoms in the form of positive ions and boron atoms in the form of negative ions in silicon.

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Рентгенівська та раманівська спектроскопія бінарних сполук кремнія $(\text{Si}_2)_{1-x}(\text{BP})_x$ G.H. Mavlonov¹, N.F. Zikrillaev¹, A.A. Usmonov¹, G.A. Kushiev¹, Kh.S. Turekeev²¹ *Tashkent State Technical University, 100095 Tashkent, Uzbekistan*² *Nukus State Pedagogical Institute, Nukus, Republic of Karakalpakstan, Uzbekistan*

У роботі досліджується взаємодія домішкових атомів фосфору та бору в кремнії за допомогою рентгенівської та раманівської спектроскопії. Було підготовлено дві групи зразків: першу групу спочатку легували атомами фосфору, а потім атомами бору; у другій групі спочатку вводили атоми бору, а потім атоми фосфору. Раманівську спектроскопію використовували для аналізу утворення бінарних сполук атомів фосфору та бору в кремнієвій матриці, а також їх оптичних, фотоелектричних та структурних властивостей. Результати показали, що атоми фосфору та бору як домішки кремнія суттєво змінюють кристалічну структуру та електропровідність. Зразки, леговані фосфором, демонстрували вищу електропровідність та фотоелектричні властивості, тоді як зразки, леговані бором, демонстрували нижчі оптичні та електричні властивості. Дані, отримані за допомогою раманівської спектроскопії, чітко продемонстрували атомні взаємодії та кристалічну структуру. Крім того, мікроструктура зразків вивчали методом скануючої електронної мікроскопії (SEM) та атомно-силової мікроскопії (ASM). SEM-аналіз виявив нерівномірний розподіл атомів бору та фосфору і нанорозмірні структури, тоді як ASM-аналіз – дрібні зміни та структурні дефекти на поверхні легованих кремнієвих матеріалів. Результати цього дослідження розширюють можливості контролю властивостей напівпровідників шляхом легування кремнію домішковими атомами та формування бінарних сполук, сприяючи розробці нових технологічних рішень та матеріалів, особливо в оптоелектроніці та сенсорних технологіях.

Ключові слова: Напівпровідник, Кремній, Бор, Фосфор, Спектр комбінаційного розсіювання, Спектрометр, Лазер, Дифузія.