

## INFLUENCE OF DIFFERENT TYPES OF RADIATION ON THE CRYSTAL STRUCTURE OF SILICON MONOCRYSTALS n-Si

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In this work, the influence of alpha particles, protons and gamma rays on the crystal structure and structural characteristics of n-type silicon (n-Si) single crystals was studied using X-ray diffraction. N-type silicon (KEF-40) was used for the study. The samples were irradiated with protons with a dose of  $9 \times 10^{14} \text{ cm}^{-2}$  with an energy of 600 keV and a current of  $1 \div 1.5 \text{ } \mu\text{A}$ , irradiated with alpha particles with a dose of  $6 \times 10^{14} \text{ cm}^{-2}$  with an energy of 800 keV and a current of  $0.5 \div 1 \text{ } \mu\text{A}$  and  $\gamma$ -<sup>60</sup>Co quanta with a flux intensity of  $\sim 3.2 \times 10^{12} \text{ quantum/cm}^2 \cdot \text{s}$ . Based on the results of X-ray diffraction analysis, it was established that distortions, vacancies and amorphization of lattice parameters that arose after irradiation lead to an increase in lattice parameters.

**Key words:** Monocrystal; Silicon; Irradiation; Alpha particles; Proton; Gamma quantum; X-ray diffraction

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### INTRODUCTION

In recent years, scientists around the world have paid great attention to research into the electrical properties and structure of semiconductors. Because the basis of modern microelectronics is semiconductor materials and various device structures based on them. Today, in the context of the rapid development of technology and technology, the creation of sensitive and resistant to external influences devices with wide application possibilities and completely new semiconductor materials that can serve as the basis for them is considered one of the urgent tasks [1-3].

In the technological processes of manufacturing semiconductor devices, semiconductor materials are subjected to various mechanical, thermal, and radiation influences. These effects, in turn, can lead to a noticeable change in the initial parameters of semiconductor materials [4,5].

Irradiation of silicon with protons and alpha particles leads to the formation of primary point radiation defects in the crystal – vacancies and associated interstitial silicon atoms (Frenkel pairs), which are generated along the ion path as a result of the development of cascades of collisions of ions with atoms of the crystal lattice. During irradiation at room temperature, especially created pairs of Frenkel disappears as a result of reciprocal annihilation, and the isolated components of the pairs, in the process of their movement, cooperate with each other and with impurity atoms of the crystal, creating more complex and stable secondary radiation defects. Secondary defects are subsequently transformed, for example, when exposed to temperature, complex complexes can decompose into components [6-7].

The main aim of this work is to investigate the effect of various types of radiation on changes in the crystal structure and structural characteristics of n-type silicon single crystals using X-ray diffraction.

As is known [8], X-ray analysis is based on the Wulff–Bragg equation, which relates the interplanar distance ( $d$ ), angle of incidence of X-rays ( $\theta$ ) and wavelength ( $\lambda$ ):

$$\lambda = 2d \sin \theta. \quad (1)$$

The main advantages of X-ray diffraction analysis are that the solid body itself is examined in an unchanged state and the result of the analysis is the direct determination of the substance or its components. X-rays examine the crystal, just the connection itself. Moreover, in the case of polymorphic bodies, X-rays make it possible to distinguish individual modifications characteristic of a given substance. To study a substance, a very small amount is required, which is not destroyed during the analytical operation [9,10]. A crystalline substance of a certain chemical composition as a result of any physical impact (mechanical, thermal) can greatly change its properties. For the most part, this is due to a change in the crystal structure (phase transformation) or distortion of this structure under the influence of external forces or internal stresses. Diffraction methods make it possible to detect the slightest changes in the state of the atomic lattice of a crystal that are not detected by other methods.

### EXPERIMENTAL PART

For the experiments, n-type silicon (KEF-40) was used, grown by the Czochralski method. The resistivity of these samples is 40 Ohm cm. The concentration of phosphorus dopant in the original n-Si single crystals was  $7.3 \times 10^{13} \div 7.1 \times 10^{15} \text{ cm}^{-3}$ .

These samples were first divided into group 3 and irradiated with alpha particles, protons and gamma rays. Samples of the first group were irradiated with alpha particles with an energy of 800 keV, a current of  $1 \div 1.5 \text{ } \mu\text{A}$  and a dose of  $6.0 \times 10^{14} \text{ cm}^{-2}$ . The samples were irradiated using the EG-5 electrostatic accelerator in the FLNP, JINR.

Samples of the second group were irradiated with protons with an energy of 600 keV at a current of  $1 \div 1.5 \text{ } \mu\text{A}$  with a dose of  $9 \times 10^{14} \text{ cm}^{-2}$ . The samples were irradiated using the SOKOL EG-2 electrostatic accelerator at the Research Institute of Semiconductor Physics and Microelectronics. The samples of the third group were irradiated at room temperature with  $^{60}\text{Co}$   $\gamma$  quanta with a flux intensity of  $\sim 3.2 \times 10^{12} \text{ quantum/cm}^2 \cdot \text{s}$ .

Investigating of n-Si samples before and after irradiation with various types of radiation source were carried out on X-ray diffractometer with a Miniflex 300/600 goniometer and a D/teX Ultra2 detector. CuK $\alpha$ 1 radiation was used, wavelength  $\lambda = 1.541 \text{ } \text{Å}$ , with an accelerating 15 mA current and 40 keV voltage on the X-ray tube. Diffraction measurements were carried out in the Bragg–Brentano beam geometry in the  $2\theta$  range from  $5^\circ$  to  $60^\circ$  continuously with a scanning speed of 10 degrees/min and an angular step of  $0.02^\circ$ .

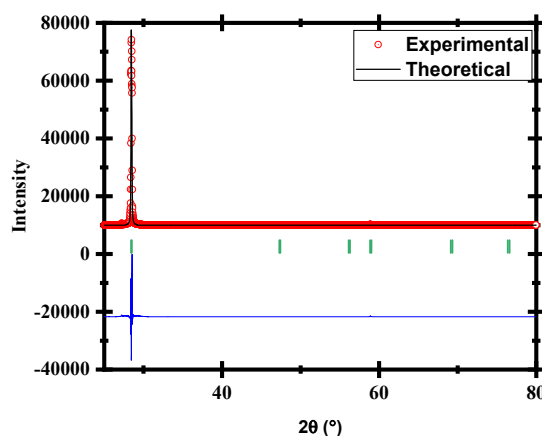
### RESULTS AND DISCUSSIONS

The influence of various radioactive methods on the structural properties of Si mono crystal was investigated. To investigate the effect of radioactivity on the structural properties of single crystals after irradiation the analysis was carried out using the X-ray method. As a result of research, it has been seen that the change of crystal lattice parameters was basically the same. Change of characteristics was studied by the Rietveld method [11], Table 1. The measurements of the material used in the experiment before and after irradiation are shown [12]. It was revealed that, after irradiation, an increase in the value of the dimensions of the lattice constant is observed. The largest jump occurred after proton irradiation.

**Table 1.** Crystal lattice parameter values determined by the Rietveld method

Name	Type of radiation	Space group	a (Å)	V (Å) <sup>3</sup>	Reliability Factors
Si	initial	F d -3 m	5.42989 (8)	160.093 (4)	Rp: 9.4 Bragg: 10.2 Rf: 15.0
Si	alpha	F d -3 m	5.43184 (10)	160.266 (5)	Rp: 10.1 Bragg: 11.0 Rf: 15.1
Si	gamma	F d -3 m	5.43368 (10)	160.429 (5)	Rp: 10.2 Bragg: 11.0 Rf: 15.0
Si	proton	F d -3 m	5.43636 (14)	160.666 (7)	Rp: 10.4 Bragg: 11.2 Rf: 15.3

After refining with the FullProf program, it was found that the diffraction peak is (111) indexed. In the initial state of the sample, the diffraction peak itself is at an angle of  $2\theta = 28.4473^\circ$  has shown (Fig. 1). Depending on the type of effect after alpha, gamma and proton radiation, the lattice of the crystal  $\Delta a_\alpha = 0.00195^\circ$ ,  $\Delta a_\gamma = 0.00379^\circ$  and  $\Delta a_p = 0.00647^\circ$  changes in parameter  $2\theta$  to  $28.4270^\circ$ ,  $28.4368^\circ$  and  $28.4127^\circ$  respectively caused a shift to the left. In Fig. 2. The shift is clearly observed.



**Figure 1.** Pre-irradiation X-ray spectrum of a Si mono-crystal

In order to see how the lattice parameters in the crystals change depending on the type of irradiation, the ratio of the lattice parameters before and after the irradiation was looked at. Increasing the value of the lattice parameters shows

a sharper change in the volume  $V/V_0$ . It can be said with certainty that after exposure to radiation, the process of amorphization and defect formation in the crystal structure increased dramatically. Since the amount of distribution of such disorders throughout the crystal increased after irradiation, it led to an increase in the value of the lattice volume parameter.

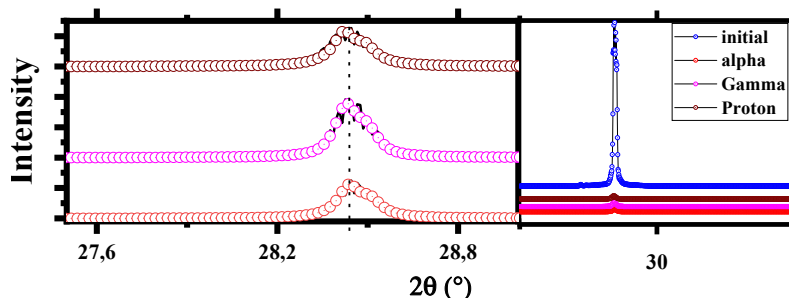


Figure 2. Shift of X-ray diffraction peaks after different types of radioactive effects

It can also be clearly seen that the changes caused by defects and lattice distortions after proton irradiation had the greatest effect on the values of the lattice parameters, and the smallest in alpha irradiation in Fig. 3.

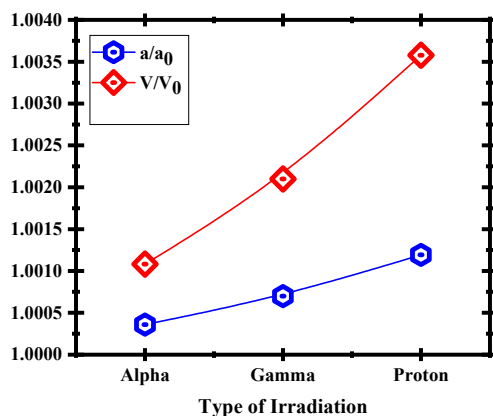


Figure 3. Characteristics of changes in lattice parameters after different types of irradiations

The crystal had a very long ordered structure before irradiation. After irradiation, this regularity decreased dramatically. By the method of integration of diffraction peaks (similarly as in this articles [13,14]), it was determined how much this change changes in which radiation. Calculations show that after alpha, gamma and proton irradiation, the long-range order in the crystal is reduced by 98.09%, 97.17%, and 97.92%, respectively. This is due to the inability of the crystal to maintain its regular structure after irradiation.

The authors [15] work with alpha-irradiated silicon monocrystalline samples with energy of 5.4 MeV. They wrote that when studying irradiated silicon samples, the presence of thin amorphized layers was observed near the surface of the samples. Irradiation of silicon with alpha particles with an energy of 5.4 MeV with doses in the range from  $4 \times 10^{10}$  to  $8 \times 10^{11}$  particles/cm<sup>2</sup> can lead to the development in the near-surface region of a compensating layer caused by excess concentrations of A-centers and complexes based on vacancies, including divacancies.

In [16], using high-resolution X-ray diffraction analysis, the transformation of radiation defects in n-type silicon crystals irradiated with protons was studied. It was shown that the proton-irradiation of silicon structures with energy of 100, 200 or 300 keV respectively with a dose of  $2 \times 10^{16}$  cm<sup>-2</sup> causes the creation of a amorphous layer 2.4 μm thick with a large crystal parameters. The layer is formed at the same time with the congestion of its own radiation defects, such as vacancies and interstitial ones.

From those results [15, 16], it can be assumed that irradiation of a silicon single crystal with various types of radiation leads to the formation of radiation defects, the creation of amorphous layers and the deterioration of the crystalline structure of silicon samples.

### CONCLUSION

The response of the Si crystal to all applied radioactive influences was similar regardless of the type of irradiation. From the results of the X-ray diffraction experiment, it was found that the distortions, vacancies and amorphization that occurred after the irradiation of the lattice parameters led to an increase in the lattice parameters. After the theoretical calculations, it was found that the increase of the lattice parameters of the crystal is up to 0.12% after proton irradiation. Disruption of the long-range regularity of the lattice due to the influence of radiation shows itself in different values depending on the type of radiation. The results show that the long order of the crystal is destroyed by more than 98 % under the influence of alpha rays. From this, we can conclude that the main reason for the increase in the size of the lattice

is the vacancies created by different types of effects, and it is assumed that as the duration of the effect changes during irradiation, these vacancies are grouped and covered in a cluster shape.

#### Conflict of Interest

The authors declare that there is no conflict of interest regarding the publication of this paper.

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#### ВПЛИВ РІЗНИХ ВИДІВ ВИПРОМІНЮВАННЯ НА КРИСТАЛІЧНУ СТРУКТУРУ МОНОКРИСТАЛІВ КРЕМНІЮ n-Si

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У цій роботі методом рентгенівської дифракції досліджено вплив альфа-частинок, протонів і гамма-випромінювання на кристалічну структуру та структурні характеристики монокристалів кремнію n-типу (n-Si). Для дослідження використовували кремній N-типу (KEF-40). Зразки опромінювали протонами дозою  $9 \times 10^{14} \text{ см}^{-2}$  з енергією 600 кеВ і силою струму  $1 \div 1,5 \text{ мкА}$ , опромінювали альфа-частинками дозою  $6 \times 10^{14} \text{ см}^{-2}$  з енергією 800 кеВ і струмом  $0,5 \div 1 \text{ мкА}$  та квантами  $\gamma$ - $^{60}\text{Co}$  з інтенсивністю потоку  $\sim 3,2 \times 10^{12} \text{ квант/см}^2 \cdot \text{с}$ . За результатами рентгеноструктурного аналізу встановлено, що спотворення які виникли після опромінювання, вакансії та аморфізація параметрів ґратки призводять до збільшення параметрів ґратки.

**Ключові слова:** монокристал; кремній; опромінювання; альфа-частинки; протон; гамма-квант; рентгенівська дифракція