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INFLUENCE OF ALPHA PARTICLES ON TECHNOLOGICAL IMPURITIES IN SILICON DOPED WITH PLATINUM

Sh.B. Utamuradova[1], D.A. Rakhmanov[1*], P.L. Tuan[2,3], A.S. Doroshkevich[2], V.A. Kinev[4], A. Tatarinova[2], R.Sh. Isayev[2], A.S. Abiyev[5]

[1]Institute of Semiconductor Physics and Microelectronics, National University of Uzbekistan, Tashkent, Uzbekistan
[2]Joint Institute for Nuclear Research, Dubna, Russia
[3]Hanoi Irradiation Center, Vietnam Atomic Energy Institute, Hanoi, Vietnam
[4]Dubna State University, Dubna, Russia
[5]Western Caspian University, Baku, Azerbaijan

Abstract. The effect of alpha particles on the concentration of optical active oxygen in silicon samples doped with platinum was studied in this work and the radiation defects that appear after irradiation with alpha particles were determined. Silicon samples were doped with platinum, followed by irradiation with alpha particles with an energy of 2 MeV, the dose was $5 \cdot 10^{14}$ cm^{-2}. Some Peaks were detected indicating the presence of various types of chemical bonds. It was determined that the introduction of platinum atoms leads to a decrease in the concentration of optically active oxygen in silicon (almost 2 times), but after irradiation with alpha particles the oxygen concentration increases. Using spectroscopic ellipsometry, the layer thicknesses were determined, which changed after doping and irradiation.

Keywords: *Semiconductor, silicon, doping, platinum, irradiation, alpha particles.*

Corresponding Author: *Dilmurod Rakhmanov, Institute of Semiconductor Physics and Microelectronics, National University of Uzbekistan, Tashkent, Uzbekistan, Tel: +998974651416, e-mail: dilmurod-1991@bk.ru*

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1. Introduction

It is known that in silicon grown by the Czochralski method and exposed to radiation, various oxygen-containing radiation defects are formed depending on the impurity composition. In addition, the presence of transition element (TE) impurities in the bulk of silicon, in particular platinum, leads to an increase in its resistance to radiation (Utamuradova *et al*., 2024; Madatov *et al*., 2024; Utamuradova *et al*., 2024a).

It is known that the main point secondary radiation defects in silicon are vacancy-impurity complexes (association of a vacancy with oxygen (A-center) and donor (E-center)), divacancy, as well as a K-center, which includes oxygen and carbon (Utamuradova *et al*., 2023; Daliev & Saparov, 2023; Utamuradova *et al*., 2023c). The impurity composition of a semiconductor can significantly influence the formation of

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radiation complexes not only through changing the rates of quasi-chemical reactions between primary radiation defects and impurities, but also due to the manifestation of additional mechanisms against the background of the main elastic mechanism of defect formation (Daliev *et al*., 2023; Utamuradova *et al*., 2024b).

The purpose of this work is to study the effect of alpha irradiation on the change in the concentration of optically active oxygen in n-type silicon single crystals doped with platinum (n-Si<Pt>) and to study radiation defect formation after irradiation with alpha particles using IR spectroscopy.

The problem of the presence of oxygen in silicon throughout the development of growth technology remains very relevant. Oxygen in silicon is the main impurity that determines the behavior of thermal donors, the thermal stability of the charge carrier lifetime, the formation of microdefects and the efficiency of gettering. Oxygen is the most interesting impurity in silicon and as a catalyst for various physical and technological effects (Ahmadova & Jabarov, 2023).

It should be noted that the optical method allows determining the oxygen content in a crystal, which is only in an atomically dispersed state. However, it is known that in silicon single crystals rotated by the Czochralski method, oxygen can be found not only in the form of Si-O-Si, but also in the form of various SiO_x precipitates that are formed during the ingot growth process. The main method for studying the state of oxygen in a silicon crystal, as well as determining its content, is the optical method (by IR absorption spectra). The optical method compares favorably with others in its higher productivity and simplicity. It is contactless, does not destroy the material, works in a fairly wide range of concentrations, sample thicknesses and is characterized by an acceptable error (Azamatov *et al*., 2023).

2. Experimental part

For the study, n-type silicon with a resistivity of 40 Ohm cm, grown by the Czochralski method, was used. In these samples, the phosphorus concentration was 4.3×10^{14} cm^{-3}. Before doping, all samples were chemically cleaned. Platinum atoms were deposited on the surface of the cleaned samples, then doped using the high-temperature diffusion method for 2 hours at temperatures T = 1200°C. Cooling of the doped samples occurred at different rates (Fistul, 2004; Utamuradova *et al*., 2023d).

The original (n-Si) and doped samples (n-Si<Pt>) were first polished with diamond paste, then irradiated with alpha particles with an energy of 2 MeV, a dose of $5 \cdot 10^{14} cm^{-2}$ using an EG-5 electrostatic accelerator.

To determine the concentration of optically active oxygen in the original and doped samples, an IR spectrometer “Shimadzu IRAffinity-1” was used in the range of 600 - 3000 cm^{-1} and in transmission mode.

An additional study of the optical properties of the sample surface was carried out using an ELLIPS-1991 spectroscopic ellipsometer at room temperature. The measurements were carried out in the wavelength range 350 ÷ 1000 nm with a step of 2 nm and the angle of incidence of the light beam was 70°. The effective medium approximation (EMA) model, the Cauchy and Urbach dispersion model and the parametric model were used to determine the layers on the surface of silicon samples.

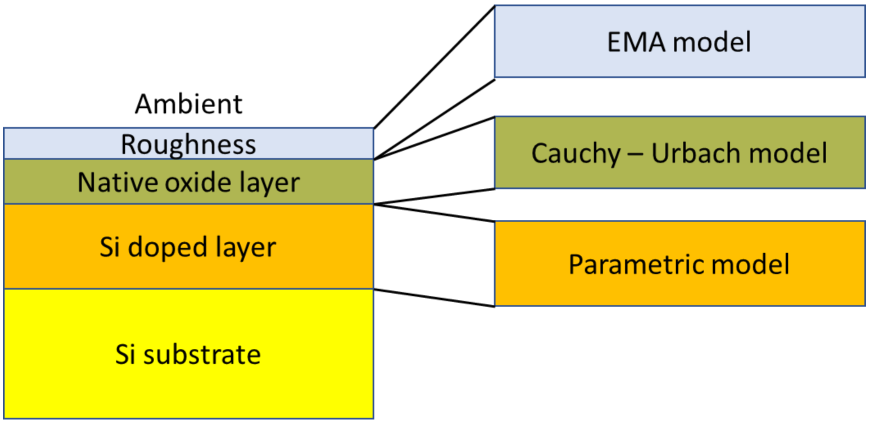

Figure 1. Models for determining layers on the surface of silicon samples

Model of Effective Medium Approximation (EMA): The layer represents the roughness that is modeled by the Bruggeman EMA of bulk material and voids. But, in this work we didn`t determine roughness of silicon samples due to polishing of surface of those samples. The Urbach and Cauchy dispersion models give the following dependences of the extinction coefficient k(λ) and refractive index n(λ) on the light wavelength λ(nm), respectively (Utamuradova *et al*., 2023e):

$$n(\lambda) = A + \frac{B}{\lambda^2} + \frac{C}{\lambda^4} + \cdots \quad (1)$$

$$k(\lambda) = \alpha e^{\beta\left(1240\left(\frac{1}{\lambda} - \frac{1}{\gamma}\right)\right)} \quad (2)$$

where A, B, C are the Cauchy coefficients, α is the amplitude of the extinction coefficient, β is the exponential factor and γ is the band edge.

3. Result and discussions

Figure 2 shows the IR spectra of the original (curve 1), platinum-doped (curve 2) and alpha-particle irradiated (curve 3, 4) samples. The measurements were carried out in a wide IR wavenumber range from 600 to 3000 cm^{-1}. In the transmission mode, some peaks were identified at wavenumbers: 2373, 1440, 1106, 950, 885, 820 and 740 cm^{-1}.

The authors (Teresa & Choi, 2010; Feifel & Lisdat, 2011) in their work determined that these peaks correspond to different types of chemical bonds: C-C (2373 cm^{-1}), C-O (1440 cm^{-1}), Si-O-Si (1106 cm^{-1}), Si-OH (885 cm^{-1}), SiO_2 (820 cm^{-1}) and metasilicate (SiO_3) bond (740 cm^{-1}). The peak that appeared at 1106 cm-1 is of greatest interest. This peak shows the concentration of optically active oxygen in silicon, which is present in a dispersed state and forms a Si-O-Si quasi-molecule with neighboring silicon atoms.

When growing silicon crystals using the Czochralski method, oxygen is the main accompanying impurity, which largely determines their electrical and optical properties (Kissinger, 2019). Essentially, oxygen is considered as a doping impurity with corresponding requirements for the level of doping and the uniformity of its distribution in the volume of a single crystal. Until recently, it was only stated that in silicon single crystals obtained by the Czochralski method, the oxygen concentration is in the range of $5 \div 9 \cdot 10^{17}$ cm^{-3} (Utamuradova *et al*., 2023a).

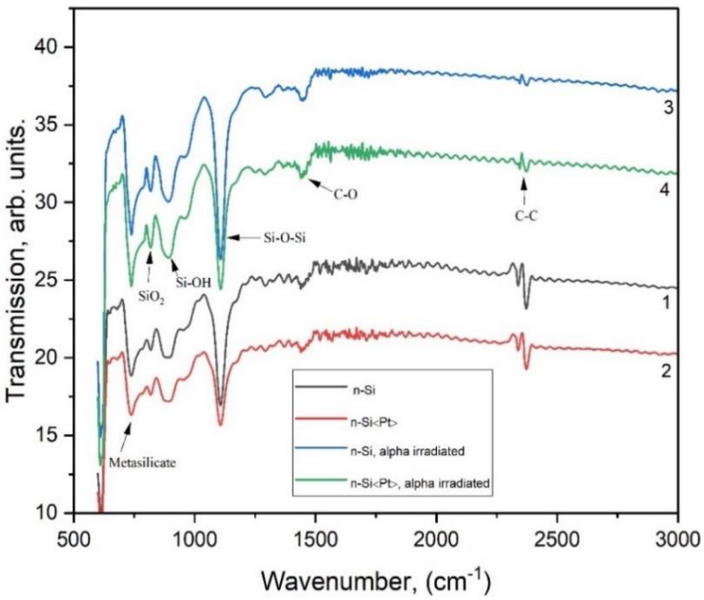

Figure 2. IR spectra of single-crystal n-type Si before (curve 1) and after (curve 2) doping with Pt and irradiation with alpha particles (curves 3 and 4, respectively)

Usually, the change in the intensity of the peaks formed in the IR spectra is associated with a change in the concentration of chemical bonds belonging to these peaks. Comparison of the IR spectra of the original and doped samples shows that doping with platinum atoms by high-temperature diffusion leads to a decrease in the concentration of optically active oxygen in silicon (almost 2 times).

Platinum is considered a transition metal with good electrical conductivity and a metal that interacts well with process impurities, in particular oxygen and carbon. During diffusion, platinum atoms interact with oxygen atoms, creating a Pt-O compound and this effect leads to a decrease in the concentration of optically active oxygen (N^{O}_{opt}) in silicon.

Next, these samples were irradiated with alpha particles with an energy of 2 MeV and a dose of $5 \cdot 10^{14}$ cm^{-2}. Comparing the IR spectra of the original and irradiated samples, we can see that after irradiation N^{O}_{opt} increases almost 1.5 times. But, in doped samples, another effect was determined, i.e. the oxygen concentration in doped and irradiated silicon is less than that of the original irradiated sample.

It is known (Utamuradova *et al*., 2023b) that irradiation of silicon structures with alpha particles leads to the creation of primary point radiation defects in the crystal, the structure of which includes vacancies. The main types of such radiation defects include vacancy-oxygen complexes (A-center), divacancy (V-V) and vacancy-phosphorus complexes (E-center). These radiation defects are considered electrically active and create deep levels in the silicon bandgap. They usually act as traps for majority charge carriers in silicon during current flow.

The authors of (Kozlov & Kozlovskiy, 2001) studied the kinetics of the appearance of interstitial carbon atoms as a result of substitution with their own interstitial atoms in silicon irradiated with alpha particles. In this work, the main parameters characterizing the rate of interaction of silicon interstices with substitutional carbon atoms are determined. The interpretation takes into account different diffusion coefficients of interstitial atoms in their singly and doubly ionized states. Other authors (Turgunov *et al*., 2021) discovered a deep level in the band gap of alpha-irradiated silicon with ionization energy Ev+0.56 eV and suggested that this level may be associated with V_2O defects, previously recognized as responsible for the inversion of the sign of the space charge in irradiated Si detectors n- type.

Based on (Utamuradova *et al.*, 2023b; Kozlov & Kozlovskiy, 2001; Turgunov *et al.*, 2021), we can assume that irradiation with alpha particles with an energy of 2 MeV leads to the creation of vacancy radiation defects in silicon and leads to an increase in the concentration of optically active oxygen in silicon due to the destruction of the Pt-O compound, which are created after doping platinum atoms.

Also, the optical properties of the original, doped and irradiated samples were further studied and some layers on the surface of these samples were determined using ellipsometric spectroscopy. Before measurements, the samples were divided into 2 groups: I - group of original and irradiated samples, II - group of doped and irradiated samples.

Using an ellipsometer, we can determine the change in polarization as light passes or reflects from a material structure. The change in polarization is shown as the amplitude ratio Ψ and the phase difference Δ. Figure 3 shows the Ψ - and Δ - spectra, as well as the optical properties of the original and irradiated samples.

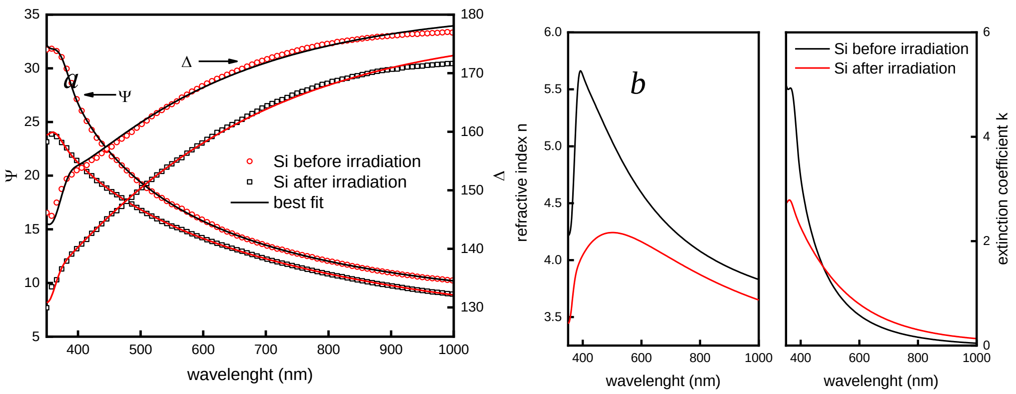

Figure 3. Ψ- and Δ- spectra (a), optical properties of Si before and after irradiation (b)

Table 1 shows parameters of oxide layers on the surface of silicon samples. It was found that in the initial samples only an oxide layer with a thickness of 5.38 nm was observed. After irradiation with alpha particles, the thickness of this layer increases to 12.52 nm.

Table 1. Parameters of oxide layers on the surface of silicon samples

No	Samples	Thickness (nm)	
		Native oxide layer	Doped layer
1	Si	5.38	0
2	Si-irradiated	12.52	0

A layer of natural oxide formed and developed on the surface of the samples. This could happen for a variety of reasons, including the roughness of the sample, the temperature of the alloying treatment and the time the sample was exposed to air. The thickness of the layer changed and we cannot establish the reasons that led to this.

Figure 4 shows the Ψ and Δ spectra and optical properties of doped and irradiated samples.

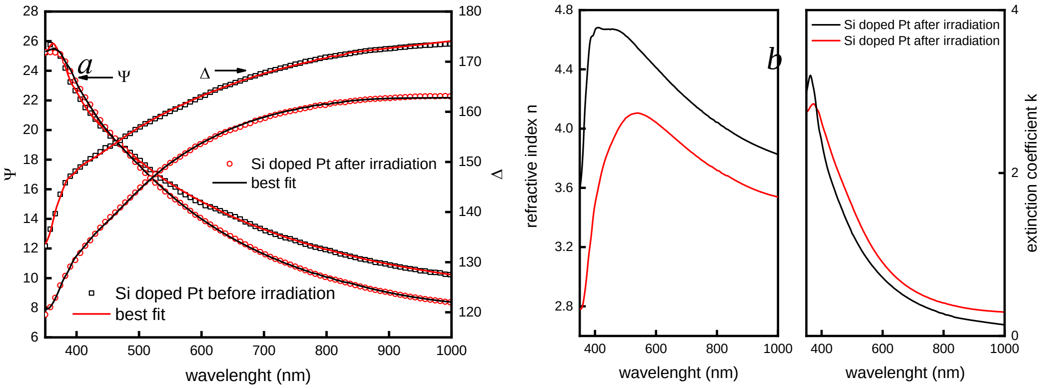

Figure 4. Ψ - and Δ - spectra (a), optical properties of n-Si<Pt> before and after irradiation (b)

From Table 2 it can be seen that after diffusion doping, in addition to the oxide layer, a layer with a thickness of 30.4 nm was formed. Further, irradiation with alpha particles with an energy of 2 MeV led to an increase in the diffusion layer to 56.33 nm. The oxide layer in these samples also increased after irradiation with alpha particles (from 8.98 nm to 14.96 nm, respectively).

Table 2. Parameters of oxide and diffusion layers on the surface of doped and irradiated samples

No	Samples	Thickness (nm)	
		Native oxide layer	Doped layer
1	Si_Pt	8.98	30.4
2	Si_Pt_irr	14.96	56.33

In general, the observed changes in native oxide layer thickness and diffusion layer in platinum-doped silicon samples before and after exposure to alpha radiation can be explained by a combination of oxidation reactions, chemical changes, dopant diffusion and surface morphology, as well as radiation-induced changes (Tuan *et al.*, 2020).

The real (ε_1) and imaginary parts (ε_2) of complex pseudodielectric functions were studied using the model method. The samples were assumed to be homogeneous and parallel. The spectra of pseudodielectric functions are calculated using the equation (Grainger & Castner, 2011):

$$\langle \varepsilon(E) \rangle = sin^2(\Phi) * \left[1 + tan^2(\Phi) * \left(\frac{1-\rho}{1+\rho}\right)^2\right] \quad (3)$$

where: Φ - angle of incidence. The value of ρ is determined by the equation: $\rho = tan(\Psi)e^{i\Delta}$ where: Ψ, Δ are ellipsometric angles.

Simultaneously with the dielectric function, the optical constants, refractive index (n) and extinction coefficient (k), which are related to ε_1 and ε_2 of the dielectric function through $\varepsilon_1=n^2-k^2$ and $\varepsilon_2=2nk$, were determined. The optical constants n and k obtained for the samples are shown in Figures 3 (for Si before and after irradiation) and 4 (for platinum-doped Si before and after irradiation).

The difference in n between samples can be explained by the difference in layer thickness. Because the thickness of the layers increases due to the increase in the optical path length and the interaction between light and materials (Guillén & Trigo, 2023). Moreover, the thickness also resulted in different interference patterns, affecting their n differently. Differences in layer thickness also affect the extinction coefficient k of samples. Two regions were observed in the k spectra. In the first region, from 350 to 380 nm for group 2 and from 350 to 470 nm for group 1, the k value is lower. This suggests that in this region the absorption of light within the material has decreased. At higher wavelengths of light (from 380 nm for group 2 and from 470 nm for group 1), the absorption mechanisms within the material may change. Thicker layers tend to exhibit higher absorption due to increased light scattering, light-matter interactions and longer optical path length, resulting in a higher extinction coefficient (Hilfiker & Woollam, 2005). In addition, the values of n, k can be influenced by factors such as the purity of the layers and the presence of defects or impurities. Higher quality material in layers with fewer defects may have higher refractive indices due to less light scattering and absorption. The observed difference in n, k spectra between samples suggests that material thickness and quality are critical factors affecting their optical properties.

4. Conclusion

Using IR spectroscopy, the change in the concentration of technological impurities in silicon was studied after doping and irradiation with alpha particles. IR spectra show that doping with platinum atoms leads to a decrease in the concentration of optically active oxygen by almost 2 times due to the creation of a Pt-O compound in silicon after doping. Further irradiation with alpha particles with an energy of 2 MeV and a dose of $5 \cdot 10^{14}$ cm^{-2} leads to an increase in N^{O}_{opt} in silicon (almost 1.5 times). This shows that alpha irradiation creates some radiation defects and destroys the Pt-O compound in silicon.

An additional study using ellipsometric spectroscopy showed that in the original samples only an oxide layer with a thickness of 5.38 nm was observed. After diffusion doping, in addition to the oxide layer, another layer with a thickness of 30.4 nm was formed. Further irradiation with alpha particles with an energy of 2 MeV led to an increase in oxide and diffusion layers on the surface of silicon samples.

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