Original Research

Raman Spectoroscopy of Silicon Single Crystals, Doped with Palladium and Irradiated by Gamma-Rays

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Abstract: In this work, the effect of γ-radiation and palladium impurities on the crystal structure of silicon samples was investigated using Raman spectroscopy. The Raman spectra of all studied samples demonstrate the presence of a main peak at ~521 cm^{-1}, corresponding to the transverse optical (TO) mode of crystalline silicon. The preservation of the position of this peak in all cases indicates that even after palladium diffusion and γ-irradiation, the silicon crystal structure remains generally stable and does not undergo complete destruction. The results show that exposure to γ-radiation leads to a noticeable increase in the low-frequency background and broadening of the main phonon peak, indicating the accumulation of radiation defects and partial amorphization of the material. The introduction of palladium significantly reduces the intensity of defect bands and stabilizes the structure, acting as a gettering and compensating element. A particularly pronounced effect is observed in samples doped with Pd at 1200 °C, where γ-irradiation has a minimal destructive effect on the lattice.

Keywords: silicon; palladium; doping; irradiation; gamma rays; Raman spectroscopy

1. Introduction

In recent decades, silicon has remained the primary material for modern semiconductor electronics due to its high purity, stable crystal structure, and ability to be precisely doped. However, a number of specialized applications, particularly in high-radiation environments (space technology, nuclear energy, radiation detectors), require a significant increase in the radiation resistance of silicon structures. Therefore, studying the mechanisms of radiation interaction with the silicon crystal lattice and finding ways to stabilize its properties remain a pressing challenge in modern semiconductor physics [1–3].

One effective approach to modifying the properties of silicon is doping it with transition metals such as palladium (Pd). Palladium can form stable complexes with lattice defects (vacancies, interstitial atoms), acting as a getter and reducing the concentration of radiation damage. Furthermore, the introduction of Pd can influence the electronic and optical properties of the material, altering the density of states and charge carrier scattering parameters. However, excess Pd or high diffusion temperatures can cause the formation of PdSi phases and localized structural defects, which requires detailed experimental analysis [4–5].

For studying structural changes caused by doping and radiation exposure, one of the most informative and non-destructive methods is Raman spectroscopy (RS). This method allows for the recording of phonon modes of the crystal lattice and is sensitive to changes in its order, defects, and

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internal stresses. Analysis of the shift, broadening, and asymmetry of Raman peaks makes it possible to identify microscopic processes occurring in the material under the influence of doping and irradiation [6–10].

This work investigates the influence of palladium atoms and γ-radiation on the structural state of n-type silicon single crystals using Raman spectroscopy. Particular attention is paid to analyzing changes in the intensity, position, and width of the main phonon peak, as well as the emergence of additional low-frequency components associated with defects and Pd–Si phases. The results obtained allow us to establish the relationship between palladium diffusion processes, radiation exposure, and the stability of the silicon crystal lattice, which is of practical interest for the creation of radiation-resistant silicon structures and devices.

2. Experimental

The object of study was n-type silicon (n-Si) with a resistivity of 40 Ohm·cm, obtained by the Czochralski method. The concentration of the phosphorus dopant in the initial single crystals was 8×10^{13}–7×10^{14} cm^{-3}. Silicon was doped with palladium by the diffusion method by depositing palladium atoms on the silicon surface in evacuated quartz ampoules at temperatures of 1100–1200 °C for 3–5 hours. Rapid cooling method (cooling rate - 400 °C /s) was used to cool the doped samples.

The original (n-Si) and doped samples (n-Si<Pd>) were irradiated with gamma quanta with an energy of 1.25 MeV at a dose of 10^7 rad using a ^{60}Co source in a gamma installation at the Institute of Nuclear Physics of the Academy of Sciences of the Republic of Uzbekistan.

The samples were studied using Raman spectroscopy using a modern Raman spectrometer "Ocean Optics" with a 785 nm excitation laser. Measurements were performed in the 0–2000 cm^{-1} range, allowing for the detection of both the fundamental phonon modes of crystalline silicon and low-frequency vibrations associated with defects and phases of palladium in the lattice.

The measurements were conducted at room temperature (T = 300 K) in a backscattering configuration. To ensure data reproducibility, each spectrum was recorded with the same accumulation time and averaging across multiple measurement series. The setup's geometry allowed signals to be acquired from the single crystal surface with high spatial accuracy, which is particularly important when analyzing inhomogeneously doped and partially irradiated regions.

Before recording spectra, the samples were thoroughly cleaned of surface contaminants and oxide layers to minimize background signal and prevent reflections. The instrument was calibrated using the standard silicon line at 521.0 cm^{-1}, ensuring high accuracy in peak position determination. The obtained spectra were processed using the OceanView software package, which includes smoothing and background correction functions. Elemental composition and micrographs of the studied samples were obtained using a JEOL JSM-IT200LA scanning electron microscope.

3. Results and Discussion

Figure 1 shows the Raman spectra of the pristine silicon (n-Si), doped samples (n-Si<Pd>), and irradiated samples. The spectrum of the pristine silicon exhibits characteristic peaks at 310 and 521 cm^{-1}, as well as a wide range of bands in the 910–1020 cm^{-1} region, corresponding to vibrations typical of the cubic structure of silicon [11,12].

The Raman spectra of all studied samples demonstrate the presence of a main peak at ~521 cm^{-1}, corresponding to the transverse optical (TO) mode of crystalline silicon. The persistence of this peak's position in all cases indicates that, even after palladium diffusion and γ-irradiation, the silicon crystalline structure remains generally stable and does not undergo complete destruction. However, changes in the peak intensity, width, and low-frequency components indicate significant processes occurring in the lattice at the microlevel [13].

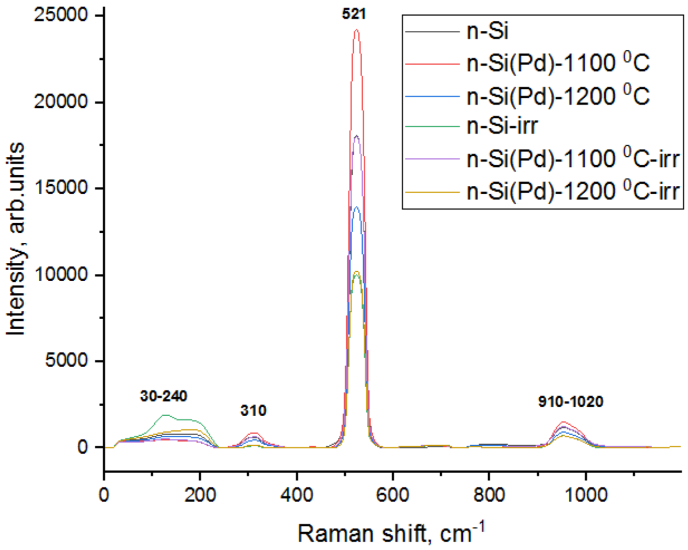
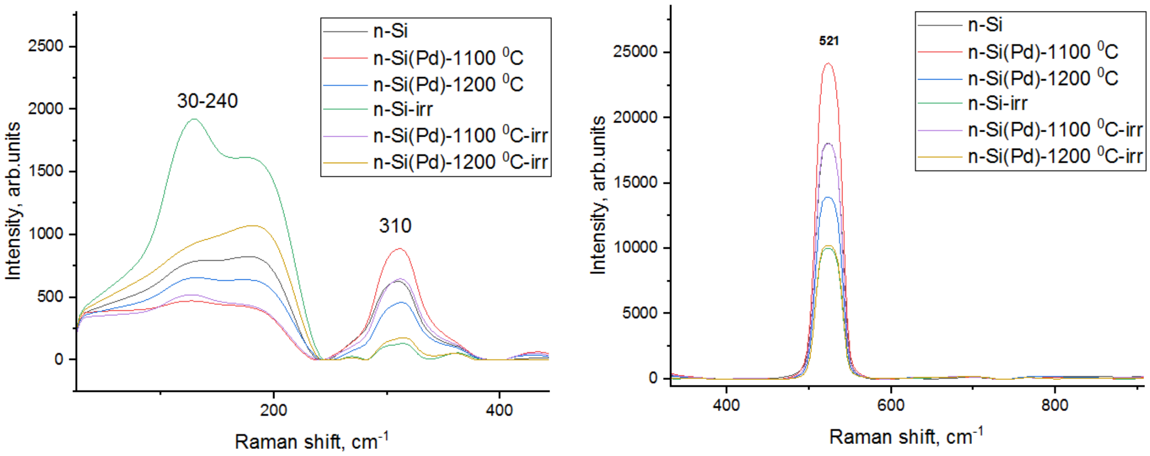


Figure 1. Raman spectra of silicon doped with palladium and irradiated with gamma-rays.

At 1100 °C, the introduction of Pd atoms into the silicon lattice does not cause a noticeable deterioration in crystallinity and does not create a new peak in the spectrum. The intensity of the main peak even increases, which may be due to increased optical polarizability due to the presence of metal atoms in the lattice [14]. Pd, possessing high chemical activity, can partially replace silicon atoms at lattice sites or occupy interstitial positions, forming local states that increase the effective scattering cross section.



(**a**) (**b**)

Figure 2. Fragments of Raman spectra of single-crystal silicon: (a) the range 30–240 cm^{-1} and around 310 cm^{-1}; (b) the main peak at 521 cm^{-1}.

With an increase in the diffusion temperature to 1200 °C, an increase in the peak width (FWHM) and a slight shift in its position towards lower wavenumbers are observed (Figure 2 (b)). This indicates the appearance of internal mechanical stresses and a partial violation of the lattice periodicity [15]. At such temperatures, the formation of palladium silicide phases (PdSi, Pd_2Si) becomes possible, which is confirmed by the appearance of weak additional bands in the region of 30–240 cm^{-1} (Figure 2 (a)). The presence of these phases leads to a local distortion of the silicon crystal lattice, an increase in the concentration of defects and a change in the distribution of charge carriers, which together are reflected in the shape of the Raman peak [16].

Elemental analysis confirmed the presence of palladium in the single crystal structure. According to the data obtained, the palladium content in the samples is 0.57 at% (or 2.82 wt.%). The energy-dispersive spectra presented in Figure 3 also indicate the presence of oxygen (1.03 at% or 1.39 wt.%) and carbon (2.32 at% or 2.86 wt.%) atoms in the studied samples in addition to palladium.

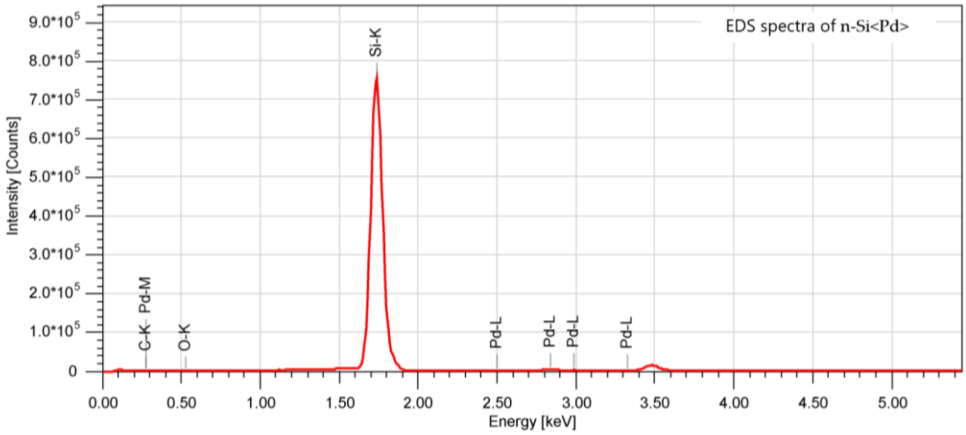
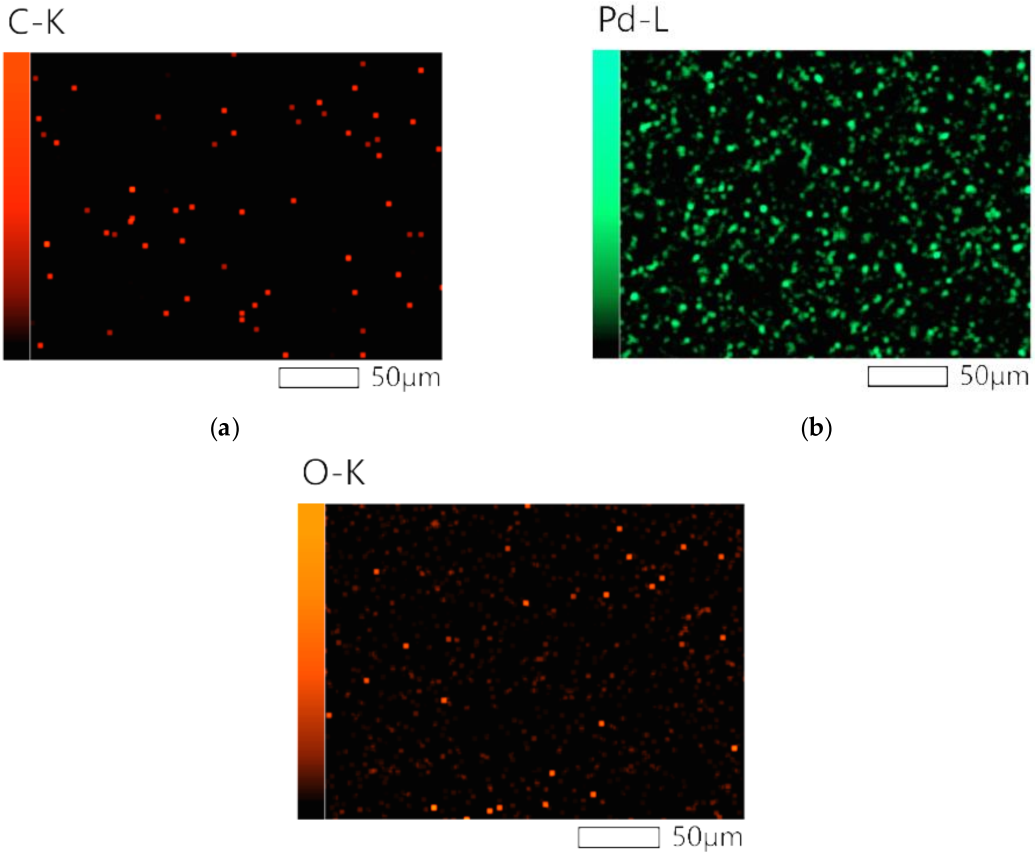


Figure 3. Energy-dispersive spectra of a silicon single crystal doped with palladium

Changing the doping temperature had virtually no effect on the concentration of palladium atoms on the silicon surface. The impurity atom distribution map (Figure 4) demonstrates that after high-temperature diffusion, palladium atoms form micro- and nanostructures that are uniformly distributed over the silicon surface.



(**a**) (**b**)

(c)

Figure 4. Micrographs of the surface of a Si single crystal after doping with Pd with distribution maps: (a) carbon(C), (b) palladium(Pd) and (c) oxygen(O).

Gamma rays have high energy and, when interacting with a silicon crystal, create primary radiation defects—vacancies, interstitial atoms, and their complexes (V–Si_i, V–O, V_2, etc.) [17,18]. The formation of such defects leads to a disruption of long-range order and the appearance of localized vibrational modes (LVM), which is manifested in an enhancement of the low-frequency component of the Raman spectrum. In the region of 30–240 cm^{-1}, broad and asymmetric bands appear, characteristic of defective and partially amorphized regions of the crystal. An increase in the FWHM of the main peak to 5.5 cm^{-1} also confirms an increase in the degree of disorder [19].

Although the intensity of the main peak remains significant, the spectrum of γ-irradiated n-Si indicates the onset of partial amorphization and a significant increase in the defect density. This effect is accompanied by a change in the optical properties, as the defects act as scattering and recombination centers for charge carriers [20].

Of particular interest is the analysis of samples in which palladium was incorporated prior to γ-irradiation. A noticeable decrease in the intensity of defect bands in the 30–240 cm^{-1} region is observed compared to pure irradiated silicon. This indicates that palladium has a stabilizing effect on the structure. Pd atoms are capable of "capturing" vacancies and interstitial atoms, forming stable complexes such as Pd–V or Pd–Si_i. Such complexes are less mobile and prevent the development of defect clusters and amorphous regions [21, 22].

At a diffusion temperature of 1100 °C, the stabilization effect is moderate, while at 1200 °C it becomes more pronounced. This can be explained by the fact that at higher temperatures, some of the palladium transforms into chemically bound states (PdSi), which effectively suppress radiation-induced defects by acting as gettering centers [23,24]. Thus, Pd not only participates in doping but also helps reduce the radiation sensitivity of silicon, which is important for the use of this material in radiation-hardened semiconductor devices.

An increase in the ratio (A_{low}/A_{TO}) (table 1) correlates well with the growth of material defects. For untreated silicon, this ratio is only 0.05, whereas after γ-irradiation it increases to 0.26. In the presence of Pd and subsequent irradiation, the value decreases to 0.13–0.16, confirming the role of palladium in suppressing radiation defects. Thus, Raman spectroscopy clearly demonstrates the evolution of the structural state of silicon as a function of diffusion temperature and irradiation dose.

Table 1. Main parameters of Raman spectra of n-Si single crystals

Samples	**Peak TO (cm^{-1})**	**FWHM (cm^{-1})**	**Intensity**	**Intensity 30–240 cm^{-1}**	**A_{low}/A_{TO}**
n-Si (initial)	521.2	4.5	100	50	0.05
n-Si<Pd> - 1100 °C	521.3	4.6	115	70	0.06
n-Si<Pd> - 1200 °C	520.9	5.2	90	110	0.12
n-Si irradiated	521.1	5.5	85	2020	0.26
n-Si<Pd>- 1100 °C irradiated	521.0	5.4	90	1400	0.16
n-Si<Pd> - 1200 °C irradiated	520.8	5.6	80	1000	0.13

4. Conclusions

A Raman spectroscopy study revealed that the structural state of n-type silicon single crystals depends significantly on palladium diffusion processes and subsequent γ-irradiation. The initial silicon samples are characterized by a narrow and intense phonon peak at 521 cm^{-1}, indicating a high degree of crystallinity and a minimal concentration of lattice defects.

After palladium diffusion at 1100 °C, the silicon structure remains predominantly ordered, but an increase in the intensity of the main peak is observed, indicating increased optical activity and the possible formation of local scattering centers. As the diffusion temperature increases to

1200 °C, a broadening of the Raman line and the appearance of additional low-frequency modes are observed, associated with the formation of PdSi phases and an increase in crystal defects.

Exposure to gamma radiation leads to a noticeable increase in the low-frequency background and a broadening of the main phonon peak, indicating the accumulation of radiation-induced defects and partial amorphization of the material. The introduction of palladium significantly reduces the intensity of the defect bands and stabilizes the structure, acting as a gettering and compensating element. This effect is particularly pronounced in samples doped with Pd at 1200 °C, where gamma irradiation has minimal destructive effect on the lattice.

Thus, the analysis confirms that palladium effectively increases the radiation hardness of silicon by binding radiation-induced defects into stable Pd–V and Pd–Si_i complexes. These results have important practical implications for the development of radiation-hardened semiconductor structures and devices designed to operate under intense ionizing radiation.

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Author Contributions: SBU conceived and designed the study, developed the methodology, supervised the research, and wrote the original draft of the paper. DAR performed the experiments, analyzed the data, and contributed to writing, reviewing, and editing the manuscript. ASA collected the data, participated in the discussion of the results, and performed the formal analysis. All authors have read and approved the final manuscript. All authors contributed to editorial changes in the manuscript. All authors have participated sufficiently in the work and agreed to be accountable for all aspects of the work.

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