

The Role of Si Self-interstitial Atoms in the Formation of Electrically Active Defects in Reverse-Biased Silicon $n^+ - p$ Diodes upon Irradiation with Alpha Particles

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Dedicated to the memory of Dr. Leonid I. Murin, who initiated this work but passed away in July 2020

Results of a study of changes in electrical characteristics of $n^+ - p$ diodes on boron-doped epi-silicon induced by irradiation with alpha particles under applied reverse bias voltages are presented. It is found that the irradiation results in a significantly lower introduction rate of carrier-compensating radiation-induced defects (RIDs) in the space charge region of the reverse-biased structures compared with those in the neutral base region and in similar diodes irradiated without bias. The dominant hole and electron emission signals in the capacitance transient spectra of the irradiated diodes are characterized and identified with energy levels of some known RIDs in moderately doped p-type Si:B. Changes in concentration of the defects are monitored after postirradiation minority carrier injection and thermal treatments. It is argued that the observed effect of the reduced concentration of RIDs in the space charge regions of the diodes is related mainly to some specific features of the silicon self-interstitials (I_{Si}): a very strong dependence of their thermal stability on the charge state and a highly enhanced mobility in p-type Si under minority carrier injection conditions. The activation energy of electron emission from the doubly positively charged state of I_{Si} is determined.

has been collected with the use of multiple experimental and modeling techniques. This has resulted in solid knowledge of the introduction rates, structure, and electronic and dynamic properties of many primary and secondary radiation-induced defects.^[1–3] It should be noted that some care should be taken when using the available information on radiation-induced processes in silicon crystals for prediction of changes in characteristics of Si-based devices, which are subjected to irradiation with high-energy particles in active regimes, i.e., either reverse or forward biased. It has been shown that there are some peculiarities in the formation of radiation-induced defects in the active regions of Si-based devices.^[4–7] Some attempts have been undertaken to explain the observed effects in the irradiated devices, which have been only partially successful.^[4,7] Many Si-based devices, such as Si particle detectors and CCD image sensors,


1. Introduction

Radiation-induced defects in silicon crystals have been extensively studied since the middle of the last century. A lot of information on the processes that occur in Si materials with different contents of impurities upon their exposure to irradiation with different high-energy particles and following heat treatments

are subjected to irradiation with high-energy particles when in the active regimes,^[3,6,7] usually under reverse bias. Therefore, a detailed understanding of radiation-induced processes in the active regions of such devices is required. In this study, we present results of a study of changes in electrical characteristics of $n^+ - p$ diodes on boron-doped epi silicon induced by irradiation with alpha particles under applied reverse bias voltages.

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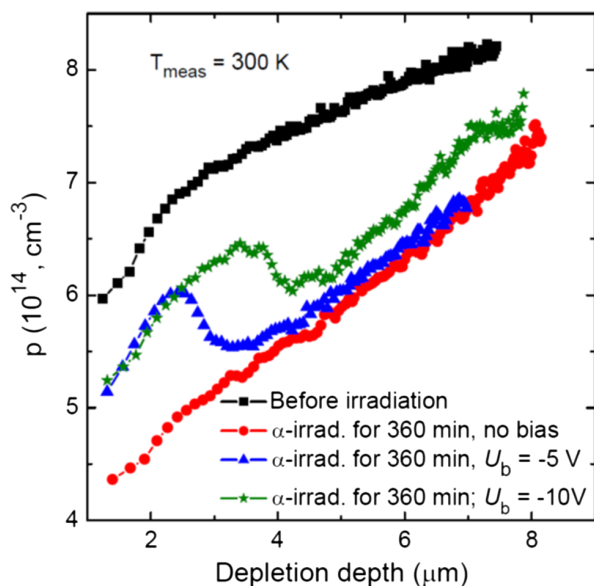


Figure 1. Spatial profiles of the hole concentration, $p(W)$, in an as-manufactured diode and in the diodes that were subjected to irradiation with alpha particles for 360 min being either unbiased or under reverse bias voltages of -5 or -10 V. The profiles have been calculated from the C - V dependencies measured at 300 K.

2. Results and Discussion

2.1. Spatial Profiles of Hole Concentration in the Diodes Subjected to Irradiation, Minority Carrier Injection, and Thermal Treatments

Figure 1 shows spatial profiles of the hole concentration, $p(W)$, in an as-manufactured diode and in diodes that were subjected to irradiation with alpha particles for 360 min being either unbiased or under reverse bias voltages of -5 or -10 V. The profiles have been calculated from the C - V dependencies measured at 300 K. The irradiation of the unbiased sample resulted in the decrease of hole concentration of about $\Delta p/p_0(W) \approx 0.35$ in the probed regions due to the introduction of carrier compensating traps. $p_0(W)$ is the hole concentration at the depth W from the n^+-p junction in the as-manufactured diode, and $\Delta p(W)$ is the decrease in hole concentration resulting from the irradiation. **Figure 1** shows that the $\Delta p/p_0(W)$ ratio for the diode, which was irradiated unbiased, is nearly constant in the probed region, so indicating the nearly uniform introduction rate of radiation-induced defects in this diode. This result is expected as the penetration depth of alpha particles with energies in the region of 5 MeV exceeds $20 \mu\text{m}$ in silicon.^[8]

The spatial profiles of the hole concentration in the diodes that were subjected to irradiation under reverse bias voltages are not uniform. There are kinks on the $p(W)$ dependencies for those diodes, the positions of which correspond to the edge of the space charge region in the diodes for the applied bias voltage. It is clear that the concentration of carrier-compensating traps is significantly lower in the space charge regions of the diodes compared with those in the neutral bulk region and in similar diodes irradiated without bias.

Figure 2 shows spatial profiles of the hole concentration in two diodes that were subjected to irradiation with alpha particles under different conditions: a) with no bias and b) with the reverse bias voltage of -10 V applied to a diode during irradiation. After irradiation, the diodes were subjected to identical subsequent treatments consisting of 1) minority carrier injection induced by forward biasing with forward current of 3.2 A cm^{-2} at 80 K for 1 min and 2) annealing at 100°C for 30 min with no bias applied. It is found that the minority carrier injection results in significant recovery of hole concentration in the whole probed region of the diode irradiated without bias, and in the bulk neutral region of the diode irradiated with the bias applied. The change of hole concentration in the region that was depleted of free carriers upon irradiation is much smaller compared to that in the bulk neutral region (**Figure 2b**). The subsequent heat treatments of the diodes at 100°C for 30 min with no bias applied did not result in significant changes in the $p(W)$ profiles for both diodes. Some small reverse recovery of the $\Delta p(W)$ values after the heat treatment in relation to the values after the minority carrier injection can be mentioned.

To understand the nature of the changes in $p(W)$ dependencies shown in **Figure 1** and **2**, we conducted DLTS measurements on the diodes subjected to irradiation, minority carrier injection, and thermal treatments.

2.2. DLTS of the Diodes Subjected to Irradiation with Alpha Particles under Different Conditions

Figure 3 shows the DLTS spectra recorded on a) a diode that was subjected to irradiation with alpha particles for 360 min being unbiased and b) a diode that was subjected to irradiation with alpha particles for 360 min under the reverse bias voltage of -10 V. The spectra for both diodes were recorded with the use of two bias/pulse sets given in the graph to characterize deep-level hole traps in different regions of the diodes. For the diode that was irradiated under bias these were 1) the region depleted of free carriers upon irradiation and 2) the neutral bulk region. In the plotted spectra, the measured $\Delta C/C_b$ values have been multiplied by the f coefficient $\{f = W_b^2/(W_b^2 - W_p^2)\}$, which takes into account depletion widths under bias (W_b) and pulse (W_p) voltages.^[9,10] The plotted $\Delta C:f/C_b$ values are proportional to ratios of concentrations of deep level traps to uncompensated shallow acceptors.

Three dominant peaks due to hole emission from traps with deep levels in the lower half of the Si gap have been detected in the DLTS spectra for both samples. The peak maxima for the used emission rate window of $e_{em} = 19.1 \text{ s}^{-1}$ are found to be at about 112, 144, and 178 K. We measured temperature dependences of hole emission rates for the detected traps and determined the activation energies for hole emission (E_{em}) and pre-exponential factors (A) from Arrhenius plots of T^2 -corrected emission rate values. The derived E_{em}/A values are $0.19 \text{ eV}/7.4 \times 10^5 \text{ s}^{-1} \text{ K}^{-2}$, $0.29 \text{ eV}/1.6 \times 10^7 \text{ s}^{-1} \text{ K}^{-2}$, and $0.365 \text{ eV}/1.2 \times 10^7 \text{ s}^{-1} \text{ K}^{-2}$ for the traps with their emission peak maxima at 112, 144, and 178 K, respectively. A comparison of the obtained results with those available in the literature on the radiation-induced defects in moderately boron-doped epi- and Cz-Si crystals allowed us to identify the detected signals with

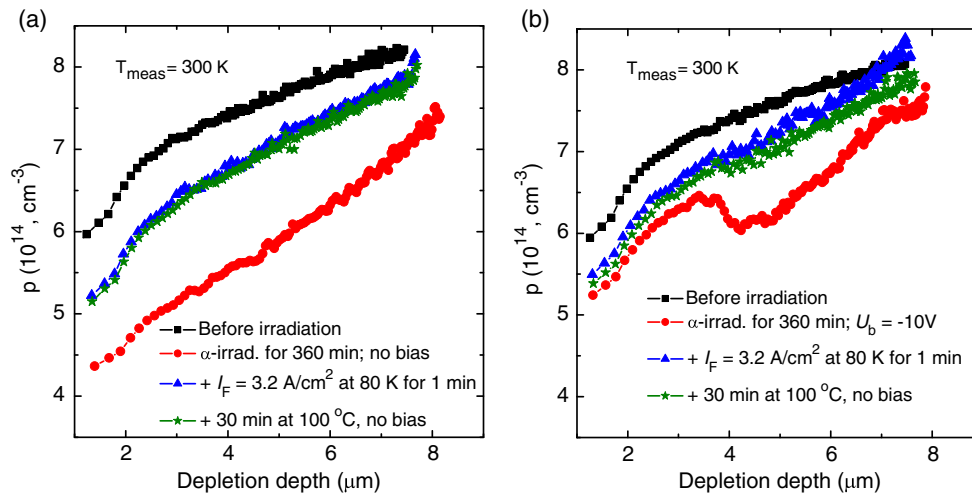


Figure 2. Spatial profiles of the hole concentration, $p(W)$, a) in an as-manufactured diode and in the same diode that was subjected to irradiation with alpha particles for 360 min being unbiased and b) in an as-manufactured diode and in the same diode that was subjected to irradiation with alpha particles for 360 min under reverse bias voltage of -10 V. Both diodes were subjected to subsequent identical postirradiation treatments: 1) minority carrier injections induced by forward biasing with forward current of 3.2 A cm^{-2} at 80 K for 1 min and 2) annealing at 100°C for 30 min with no bias applied. The profiles have been calculated from the C – V dependencies measured at 300 K .

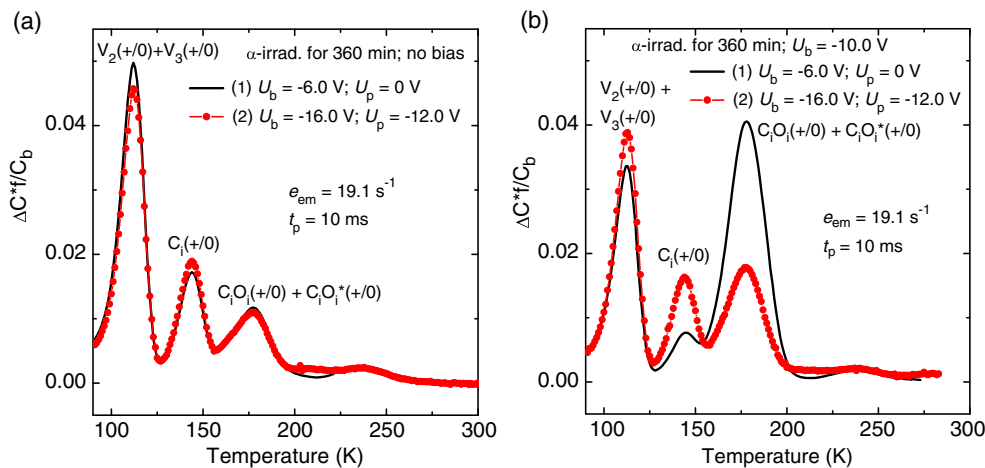


Figure 3. DLTS spectra of a) a diode that was subjected to irradiation with alpha particles for 360 min being unbiased and b) a diode that was subjected to irradiation with alpha particles for 360 min under a reverse bias voltage of -10 V . The spectra for both diodes were recorded at two bias/pulse conditions given in the graph to characterize deep-level traps in different regions of the diodes. For the diode that was irradiated under bias, these were 1) the region depleted of free carriers upon irradiation and 2) the neutral bulk region. In the plotted spectra, the measured $\Delta C^*/C_b$ values have been multiplied by f coefficient, which takes into account depletion widths under bias and pulse conditions.^[9,10] The plotted $\Delta C^*/C_b$ values are proportional to ratios of concentrations of deep level traps and uncompensated shallow acceptors.

donor levels of divacancy (V_2) and trivacancy (V_3), interstitial carbon atom (C_i), and a complex consisting of interstitial carbon–interstitial oxygen atoms in two configurations (C_iO_i and $C_iO_i^*$).^[2,3,8,11–15]

The magnitudes of the DLTS peaks due to these defects are similar in different regions of the diode, which was irradiated without bias (Figure 3a). This indicates nearly uniform introduction rates of these defects in the probed regions. It should be noted that the concentrations of $V_2 + V_3$ significantly exceed those of the C_i and C_iO_i complexes in all the probed regions of this sample. In contrast, magnitudes of the DLTS peaks

due to the $V_2 + V_3$, C_i , and C_iO_i defects differ in different regions of the diode that was irradiated with an applied reverse bias voltage (Figure 3b). In the region that was depleted of free carriers upon irradiation, the magnitude of the peak due to the C_iO_i complexes is stronger compared to those due to $V_2 + V_3$ and C_i . Further, the concentration of the C_iO_i complexes in this region significantly exceeds its concentration in the deeper bulk region, which was neutral during irradiation. The observed variations in the concentrations of the $V_2 + V_3$, C_i , and C_iO_i defects cannot, however, explain the unusual characteristics of the $p(W)$ profiles of the irradiated samples shown in Figure 1.

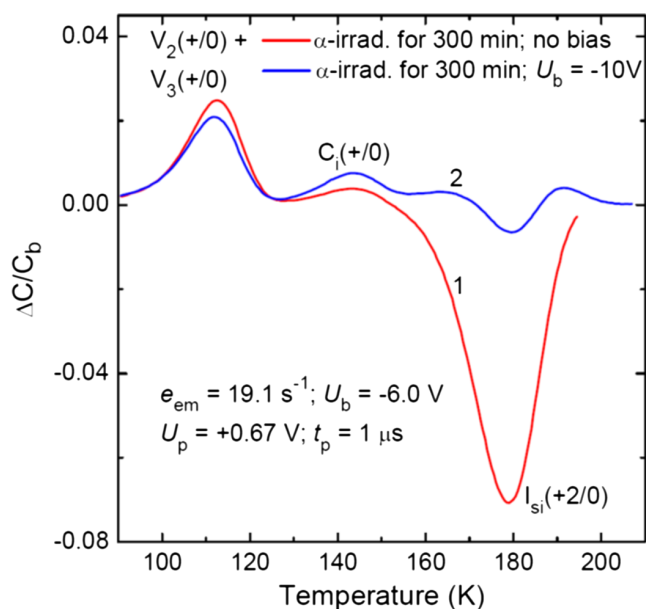


Figure 4. DLTS spectra of 1) a diode that was subjected to irradiation with alpha particles for 300 min being unbiased and 2) a diode that was subjected to irradiation with alpha particles for 300 min under a reverse bias voltage of -10 V. The spectra were recorded with the application of a pulse voltage of $+0.67$ V for injection of electrons and detection of electron traps with energy levels in the upper half of the gap.

We have attempted to detect radiation-induced traps with deep levels in the upper half of the Si gap in the irradiated diodes. **Figure 4** shows the DLTS spectra, which were recorded with a pulse voltage of $+0.67$ V aimed at injection of electrons and recharging of traps in the upper half of the gap, for two irradiated diodes. The first one was subjected to irradiation with alpha particles for 300 min being unbiased, and the second one was subjected to the same irradiation under a reverse bias voltage of -10 V. The spectra for these two diodes differ significantly. In the spectrum of the diode that was irradiated unbiased, a strong negative peak with its minimum at about 179 K occurs. This peak is related to electron emission with the activation energy of about 0.43 eV relative to the conduction band edge (**Figure 5**) from a trap with concentration that significantly exceeds the concentrations of all other radiation-induced traps detected in the DLTS spectra. It should be noted that the magnitude of the peak due to this trap can be considered only as a measure of the minimum limit of the trap concentration because of the possible incomplete occupation of the trap with electrons during the DLTS filling pulse of positive voltage for several reasons.^[9] It is further found that the obtained value of the apparent capture cross-section of electrons by the trap, $1.2 \times 10^{-13} \text{ cm}^2$ (**Figure 5**), is rather large, so indicating a donor character of the trap. The concentration of the trap is significantly smaller in the diode that was irradiated with the reverse bias applied during irradiation, i.e., in the region depleted of charge carriers upon irradiation. Bearing in mind the donor character of the trap, and so its hole compensation nature, it is possible to explain the peculiar characteristics of the $p(W)$ profiles of the irradiated samples shown in **Figure 1** by different

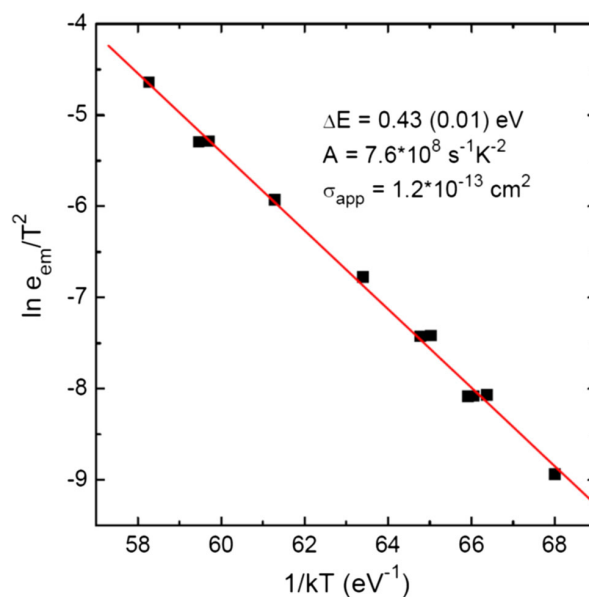


Figure 5. Arrhenius plot of the electron emission rates from the dominant deep-level trap induced in the bulk neutral regions of the n^+p diodes by irradiation with alpha particles.

introduction rates of the defect with $E_{em} = E_c - 0.43$ eV in the diodes subjected to irradiation with alpha particles under different conditions.

2.3. DLTS of the Diodes Subjected to Post-Irradiation Minority Carrier Injection and Thermal Treatments

It has been argued by Mukashev et al. that silicon self-interstitials (I_{Si}) are one of the dominant electrically active defects introduced by irradiation with alpha particles and protons at temperatures below 300 K into p-type Si crystals.^[16] Mukashev et al. have assigned the DLTS signal with $E_{em} = E_c - 0.39$ eV in the irradiated Si samples to electron emission from the doubly positively charged state of I_{Si} .^[16] It was further found that at equilibrium conditions I_{Si}^{+2} can survive in p-Si for a rather long time at room temperature. The activation energy of the I_{Si} disappearance upon thermal treatments was estimated as 1.1–1.3 eV.^[17] The disappearance of I_{Si} upon thermal treatments of p-type Si crystals was found to result in the appearance of interstitial atoms of acceptor impurities (B, Al, Ga) and carbon.^[16,17] Another remarkable feature of I_{Si} is their extremely strong sensitivity to injection of minority carriers (electrons),^[16] which was mentioned in early experiments on introduction of defects into Si crystals by irradiation with electrons with energies in a few megaelectronvolt range.^[18] Upon minority carrier injection treatments, Si self-interstitials disappeared even at cryogenic (≈ 4 K) temperatures.^[18] It was argued that the minority carrier injection could result in some athermal mechanisms of I_{Si} diffusion.^[18–20]

It appears that the electron trap with $E_{em} = E_c - 0.43$ eV, which we detected in the DLTS spectra (**Figure 4**), resembles the trap that was assigned earlier to I_{Si} . To get further support for this assumption, we conducted minority injection and

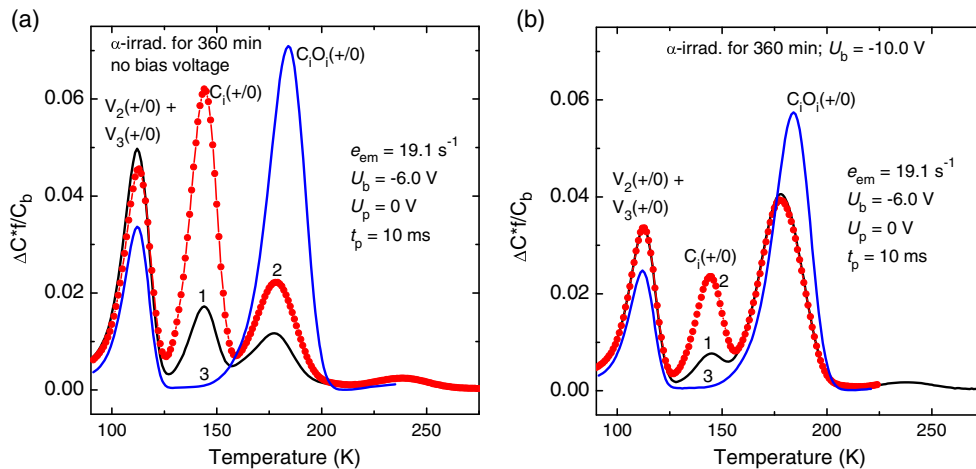


Figure 6. DLTS spectra of a) a diode that was subjected to 1) irradiation with alpha particles for 360 min being unbiased and b) a diode that was subjected to 1) irradiation with alpha particles for 300 min under a reverse bias voltage of -10 V. Both diodes were subjected to subsequent identical postirradiation treatments: 2) minority carrier injections induced by forward biasing with forward current of 3.2 A cm^{-2} at 80 K for 1 min and 3) annealing at 100°C for 30 min with no bias applied.

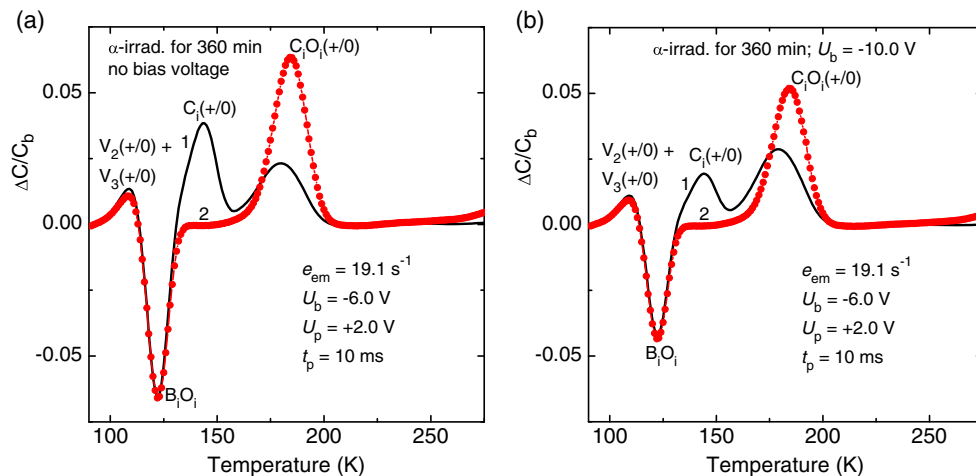


Figure 7. DLTS spectra of a) a diode that was subjected to irradiation with alpha particles for 360 min being unbiased and b) a diode that was subjected to irradiation with alpha particles for 300 min under a reverse bias voltage of -10 V. Both diodes were subjected to subsequent identical postirradiation treatments: 1) minority carrier injections induced by forward biasing with a forward current of 3.2 A cm^{-2} at 80 K for 1 min and 2) annealing at 100°C for 30 min with no bias applied. The spectra were recorded with the application of a pulse voltage of $+2.0 \text{ V}$ for injection of electrons and detection of electron traps with energy levels in the upper half of the gap.

thermal treatments of the diodes irradiated with alpha particles at different conditions. The DLTS spectra recorded after those treatments are shown in **Figure 6** and **7**. It was found that the injection treatment (forward biasing with forward current of 3.2 A cm^{-2} at 80 K for 1 min) resulted in the complete disappearance of the trap with $E_{\text{em}} = E_{\text{c}} - 0.43 \text{ eV}$ and to the introduction of C_i and B_iO_i traps into the samples. The concentrations of the introduced C_i and B_iO_i traps were significantly higher in the diodes (regions) that were irradiated without bias (were neutral upon irradiation). The subsequent heat treatment of the diodes at 100°C for 30 min results in the disappearance of C_i and introduction of the C_iO_i defect in the most energetically favorable configuration. Some decrease in the magnitude of the peak due to the $\text{V}_2 + \text{V}_3$ defects upon the thermal treatment is

mainly related to the transformation of V_3 from the planar $\langle 110 \rangle$ configuration, which possesses the donor level at $E_{\text{v}} + 0.19 \text{ eV}$, to the fourfold-coordinated configuration with the only acceptor level at $E_{\text{c}} - 0.07 \text{ eV}$.^[15,21] So, the results obtained confirm the suggestion about assignment of the trap with $E_{\text{em}} = E_{\text{c}} - 0.43 \text{ eV}$ to electron emission from the doubly positively charged state of I_{Si} .

2.4. Discussion and Conclusions

The results obtained from the DLTS measurements allow us to explain the peculiarities in the $p(W)$ dependencies for the diodes irradiated under different conditions (Figure 1). In the unbiased diodes, the irradiation with alpha particles at 290 K

results in the effective introduction of separated vacancies and interstitials. Vacancies are highly mobile at these conditions and most likely are trapped by interstitial oxygen atoms.^[18] The resulting vacancy–oxygen (V–O) complex possesses an acceptor level at $E_c - 0.17$ eV,^[1–3,18] which has not been detected in the recorded DLTS spectra. It should be noted that the introduction of the V–O complex does not result in the removal of holes in p-type Si crystals. Si self-interstitials created by the irradiation in the neutral regions of the diodes are relatively stable, and, because they are in the doubly positively charged state in p-type Si, I_{Si}^{+2} is the main defect responsible for the effective removal of holes from these regions.

The radiation-induced processes in the space charge regions of the reverse-biased diodes differ from those in the neutral regions. In these regions, the electron–hole pairs created upon the irradiation are effectively separated by the electric field and the separated electrons and holes drift. Holes drift in the field to the bulk region, and electrons drift to the n^+ emitter. The drifting electrons are attracted by I_{Si}^{+2} , which results in charge state change of Si self-interstitials and promotion of their diffusion. Upon diffusion, the I_{Si} atoms interact with substitutional carbon atoms and other defects, so their concentration in the space charge regions of the irradiated diodes is significantly lower than in the neutral regions (Figure 4). Because of their donor nature, the I_{Si} atoms are the main carrier-compensating defects in p-type Si, so their reduced concentration in the space charge regions results in the reduced removal of holes in these regions (Figure 1). It is likely that the mobile I_{Si} atoms also interact with vacancy-related defects (V–O and divacancies) in the space charge regions upon irradiation. These interactions result in the annihilation of separated vacancies and I_{Si} atoms and therefore in the reduced concentrations of all the radiation-induced defects in the space charge regions. This is manifested by the smaller magnitudes of the DLTS peaks due to the radiation-induced defects in these regions compared to those in the neutral regions (Figure 6 and 7).

3. Experimental Section

The experimental results in this work were obtained by means of junction capacitance measurements (capacitance–voltage dependences and deep level transient spectroscopy (DLTS)) on n^+p – p^+ diodes.^[9] Samples for the study were prepared from boron-doped epi-Si ($\rho \approx 20 \Omega \text{ cm}$), which was grown on highly B-doped ($\rho \approx 0.005 \Omega \text{ cm}$) bulk Czochralski-grown Si (Cz-Si) wafers. The thickness of the epi layer was $\approx 35 \mu\text{m}$. n^+p – p^+ diodes were formed by implantation of phosphorus ions with subsequent annealing at 1150°C in a nitrogen/oxygen gas ambient. The n – p junction was located at about $8 \mu\text{m}$ from the surface. Oxygen concentration in the epi layers was determined from the rate of transformation of the divacancy to the divacancy–oxygen (V_2O) defect.^[11,22] The oxygen concentration was close to $2.5 \times 10^{17} \text{ cm}^{-3}$ in all the epi-Si samples. The carbon concentration was below the detection limit of $5 \times 10^{16} \text{ cm}^{-3}$. Irradiation with alpha particles from a surface source was performed at about 290 K. The particle energies were 5.144 and 5.157 MeV. The fluence rate was $\approx 1 \times 10^7 \text{ cm}^{-2} \text{ s}^{-1}$. The damage distribution for this kind of irradiation source was described earlier.^[8] One set of the samples was irradiated with a reverse bias voltage of either -5 or -10 V applied to the diodes. Another set was irradiated with the diodes being unbiased. Thermal anneals of the irradiated structures were conducted in a furnace in a dry N_2 ambient.

The spatial distributions of the majority carrier (hole) concentration and electric field in the diodes were determined from measured dependencies of junction capacitance of the diodes on applied voltage (C–V dependencies) using the standard analysis for a sharp asymmetric n^+p junction.^[9] DLTS measurements on the irradiated diodes were usually conducted with two sets of bias-pulse voltages to probe and compare the deep-level traps created upon irradiation in the space charge and neutral regions of the devices. DLTS measurements with the application of forward bias voltages were also conducted for the detection of radiation-induced electron traps with energy levels in the upper half of the bandgap.^[9]

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Conflict of Interest

The authors declare no conflict of interest.

Data Availability Statement

Data that support the findings of this study are available from the corresponding author upon reasonable request.

Keywords

alpha particles, annealing, defects, deep level transient spectroscopy, irradiation, n^+p diodes, silicon

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