Research Report

Impact of Carbon Impurities in Silicon PIN Diodes on Electrical Dynamic Characteristics

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ABSTRACT The impact of carbon impurities in helium-irradiated silicon PIN diodes on the electrical dynamic characteristics was investigated with respect to the reliability of power devices and electrical power transformer systems. The dynamic avalanche phenomenon was observed under conditions of high carbon concentration during the reverse recovery period, and deep level transient spectroscopy (DLTS) measurements confirmed a higher hole-trap concentration at $E_T = E_V + 0.35$ eV. The dynamic avalanche phenomenon at a higher hole-trap concentration of $E_T = E_V + 0.35$ eV was predicted by device simulation taking into account the Shockley-Read-Hall (SRH) model. Cathode luminescence (CL) measurements indicated that hole-traps at $E_T = E_V + 0.35$ eV were attributable to a C_iO_i complex. First-principle calculations based on density functional theory (DFT) suggest that C_iO_i complexes form from carbon impurities during the irradiation processes, and C_iO_i possibly acts as a hole-trap center. These results suggest a mechanism by which carbon impacts the electrical dynamics, and reveal that control of the carbon impurity concentration in helium-irradiated silicon PIN diodes has a significant effect on the electrical dynamic characteristics.

KEYWORDS Silicon Power Device, PIN Diode, Reverse Recovery, Dynamic Avalanche, Hole-trap, Carbon Impurity, Hybrid Vehicle

1. Introduction

Considering present day environmental issues, the development of viable and effective technologies that save energy and reduce carbon dioxide emissions is a pressing global task. Toyota Motor Corporation has developed three generations of remarkably fuel-efficient hybrid vehicles (HV) and is working to further increase their popularity.(1-3) HVs have three basic electrical components: a battery, motor and power control unit (PCU). The PCU transfers electrical power from a DC battery to an AC motor and/or from an AC generator to a DC battery. Moreover, the Toyota Hybrid System II (THS II), first seen in second generation HVs, has a boost converter to achieve high power output.(2) **Figure 1** shows an equivalent circuit of a PCU, where the basic circuit of inverters and converter combines a two-terminal rectifier and a three-terminal switching device.

Most HVs to date use insulated gate bipolar transistors (IGBT) and PIN diodes as switching devices and rectifiers, respectively, and these power devices have been fabricated mainly from silicon (Si) crystal substrates. Recently, there has been active research into wide bandgap semiconductors made of materials such as silicon carbide (SiC) and gallium nitride (GaN) as next generation power devices.(4-7) On the other hand, further research and development of silicon power devices is also important for continued progress. A significant reduction in the power loss of Si-IGBTs has been achieved by extensive research and development efforts,(8-12) and various immunities related to device reliability, such as short circuit immunity, have been studied.(13-16) Moreover, it was recently predicted that the low loss limit of Si-IGBTs will approach that of the SiC-MOSFET.(17,18)

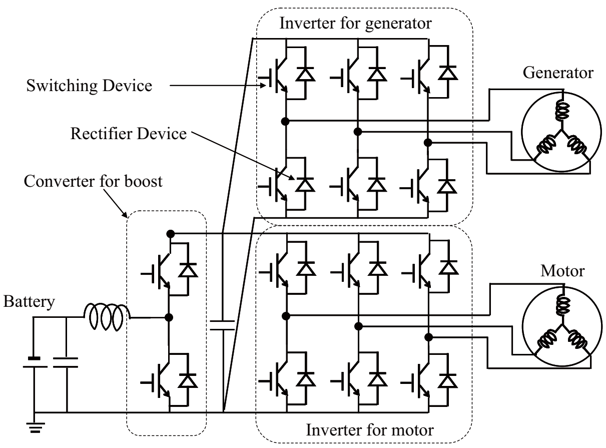

Fig. 1 Equivalent circuit of a PCU.

Therefore, there is much ongoing research related to silicon power devices. With Si PIN diodes, most studies have focused on technical issues related to electrical dynamics, because a rapid current transient results in high peak voltage, which affects device and system reliability.(19-21) Various technical approaches to soften the rapid current transient have been reported,(22-24) and the one that has been recognized as the most useful and powerful technique is helium irradiation, due to control of the local carrier lifetime in PIN diode depth profile.(22) In addition, other electrical dynamics, such as impact avalanche transit time (IMPATT), oscillation, and dynamic avalanche, have been studied recently.(25-27) In this paper, we focus on the dynamic avalanche phenomenon as an important electrical dynamic characteristic related to device and system reliability; however, there have been very few reports investigating the direct relationship between dynamic avalanching and impurities in silicon. In this study, we focus on the impact of impurities in helium-irradiated silicon crystal on the dynamic avalanche.(28,29)

2. Theory

Figure 2 shows a current and voltage waveform to discuss simple electrical dynamic characteristics schematically. While the diode current changes from on-state to off-state, the diode on-state current, i.e., forward current I_F flowing through the PIN junction, changes to a reverse current. The diode voltage, where V_{KA} is the voltage between the cathode and anode terminals, increases rapidly. Once the reverse current peaks, the transient state recovers to the off-state. The combination of the rapid transient in the reverse-recovery current I_{RR} and parasitic inductance leads to a high peak voltage. Once the reverse recovery current turns entirely to the off-state, the diode voltage also turns to the off-state. These electrical dynamic characteristics are generally called reverse-recovery characteristics. The Energy Band theory and Shockley-Read-Hall (SRH) model are very useful to discuss electrical dynamic characteristics.(30) **Figure 3** shows the basic carrier trap processes, illustrating the single-energy-level carrier generation-recombination center for electrons and holes, and the capture-emission center for holes, in which only one trapping energy level is present in the bandgap. The carrier trap at the deep energy-level readily acts as a generation-recombination center, and the carrier trap at the shallow energy-level readily acts as a capture-emission center. In considering dynamic avalanching, the minority carrier capture mechanism in the i-region plays a key role, and the i-region is slightly an n-type layer for PIN diodes; therefore, hole-capture by the trap center is an important mechanism. The hole-capture rate is given by:

$$r_{h\_c} = \sigma_h v_{th\_h} p_{inj} N_{hT} f_T , \cdots\cdots\cdots\cdots\cdots\cdots (1)$$

where σ_h is the hole-capture cross-section, v_{th_h} is thermal velocity for the hole, p_{inj} is the hole concentration injected into the i-region, N_{hT} is the hole trap concentration, and f_T is the electron occupation probability of the trap. Under equilibrium conditions, f_T is expressed by the Fermi-Dirac distribution function, and the rates of hole capture and emission are balanced. Consequently, the hole-capture time is given by:

$$t_{h\_c} \propto (\sigma_h v_{th} n_i)^{-1} \exp\{-(E_i - E_T)/kT\} , \cdots\cdots (2)$$

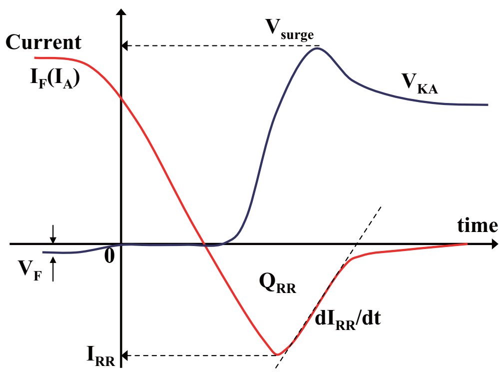

Fig. 2 Current and voltage waveform during p-in diode reverse-recovery.

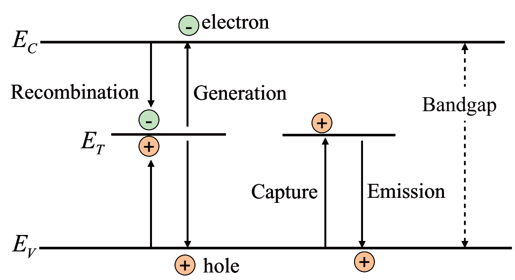

Fig. 3 Schematic illustration of carrier trap processes.

where k is the Boltzmann constant, n_i is the intrinsic carrier concentration, and E_i is the Fermi level of the intrinsic semiconductor, which generally lies very close to the middle of the band-gap. The hole-capture time is basically proportional to the energy level of the hole trap (E_T) and temperature (T), although f_T is also dependent on the injected carrier concentration, and the mechanism is more complicated under transient-state non-equilibrium conditions.

The impact ionization and electric field have to be considered in avalanche multiplication. The electron-hole pair generation rate G_{ii}, from impact ionization is given by:

$$G_{ii} = \alpha_n n v_n + \alpha_p p v_p , \quad \cdots\cdots\cdots\cdots\cdots\cdots (3)$$

where n and p are the electron and hole concentrations, v_n and v_p are electron and hole saturation velocities, and α_n and α_p are electron and hole impact ionization rates defined as the number of electron-hole pairs generated by the electrical carrier per unit distance traveled. Both α_n and α_p are strongly dependent on the electric field. A physical expression for the ionization rate is given by:

$$\alpha(\mathrm{E}) = (q\mathrm{E}/E_{I\_eff}) \exp\{-\mathrm{E}_I / [\mathrm{E}(1+\mathrm{E}/\mathrm{E}_p] + \mathrm{E}_{kT}\} , \quad \cdots\cdots\cdots\cdots\cdots (4)$$

where E_{I_eff} is the high-field effective ionization threshold energy, and E_{kT}, E_p and E_I are threshold electric fields for carriers to overcome the decelerating effects of thermal, optical-phonon and ionization scattering, respectively.(31) During the reverse-recovery period, V_{KA} rises and electron-hole pairs are swept out through each electrical terminal; however, holes captured by trap centers may remain in the high electric field region of the PIN diode. Similarly, electrons may analogously remain due to the electron-trap, but in the case of a higher hole-trap concentration than the electron-trap concentration, the effective donor concentration increases, because the hole captured by the trap center temporarily acts as a positive charge, as follows:

$$N_{D\_eff} \propto N_{D\_init} + \sum_n N_{hTn} f_{Tn} , \quad \cdots\cdots\cdots\cdots (5)$$

where N_{D_eff} is the effective donor concentration in the i-region during reverse-recovery with high V_{KA}, N_{D_init} is the initial donor concentration in the i-region, N_{hTn} is the *nth* hole-trap concentration, and f_{Tn} is the electron occupation probability of the *nth* trap. An increase in the effective donor concentration results in a high electric field. These theoretical equations indicate that hole-traps act as temporary positive charge centers that increase the electric field in the PIN diodes, and the generation probability of a dynamic avalanche during the reverse-recovery period increases because of the hole-traps. According to previous reports regarding the hole-traps in silicon crystal, for silicon irradiated using, for example, electron, proton and helium irradiation, hole-traps have been attributed to a complex related to carbon impurities.(32-34) The helium irradiation technique is useful to soften the rapid transient of a reverse recovery current, but in the light of theories and previous reports it would also be effective to achieve high reliability in power devices when investigating the impact of carbon impurities on the electrical dynamic characteristics of helium-irradiated silicon PIN diodes.

3. Results and Discussion

To investigate the effect of carbon impurities in helium-irradiated silicon PIN diodes on the electrical dynamic characteristics, two PIN diode test samples with different carbon concentrations were prepared. The wafers used were neutron transfer doping-magnetic Czochralski (NTD-MCZ) substrates that were irradiated with helium at an energy of 23 MeV in the latter stage of the PIN diode fabrication process. The two different PIN diodes were labeled samples A (low carbon concentration) and B (high carbon concentration). The carbon impurity rates for samples A and B were at a concentration of $< 10^{15}\mathrm{cm}^{-3}$ and from 10^{15}– $10^{16}\mathrm{cm}^{-3}$, respectively, during the growth stage of the MCZ substrates. The electrical dynamic characteristics, i.e. reverse recovery characteristics, were examined using the conventional double-pulse method at room temperature. As a result, voltage clumping was observed in sample B (high carbon concentration) during the reverse recovery period, which indicates dynamic avalanching, and secondary oscillation in the voltage and current waveform was observed, as shown in **Fig. 4**. By contrast, no anomalous phenomena were observed in sample A (low carbon concentration), as shown in **Fig. 5**. These results confirm that the dynamic avalanche phenomenon is significantly dependent on the concentration of carbon impurities in silicon.

To evaluate the relation between carbon impurities in silicon and the hole-traps, deep level transient spectroscopy (DLTS) measurements were performed with a conventional temperature scan using the pulse minority carrier injection method.[35] **Figure 6** shows the measured DLTS spectra of hole-traps for the two samples. The two main peaks, H1 and H2, can be attributed to hole-traps at $E_T = E_V + 0.25$ eV and $E_T = E_V + 0.35$ eV, respectively.[36] These energy levels extracted from Arrhenius plots are in good agreement with other reports.[32-34] Comparison of the DLTS results indicates that the H2 peak of sample B is higher than that of sample A. The peak height is quantitatively proportional to the hole-trap concentration. Thus, the hole-trap concentration at $E_T = E_V + 0.35$ eV of sample B was higher than that of sample A, which implies that the difference in hole-trap concentration at $E_T = E_V + 0.35$ eV between samples A and B is due to the difference of carbon concentration in the silicon. To interpret the combined results of the reverse recovery characteristics and DLTS measurements, the dynamic avalanche generation observed with higher carbon concentration is due to a higher hole-trap concentration. The influence of the hole-trap at $E_T = E_V + 0.35$ eV was examined by device simulation. The reverse-recovery characteristics were simulated by taking account of the SRH model and the hole-trap was specified at an energy level of $E_T = E_V + 0.35$ eV as a neutral hole-trap. Simulations were executed by varying the hole-trap concentration and keeping the capture coefficient constant. The simulation set-up conditions meant that the recombination ratio was constant, so that the reverse recovery charge was kept constant. Other simulation conditions, such as the PIN diode structure, temperature, bias set and initial donor concentration, were modeled on experimental conditions. The simulation results are shown in **Fig. 7**; note that the peak surge voltage could be suppressed if the hole-trap concentration was controlled to within the optimum range.[36] Under higher hole-trap concentration (N_{ht} = 20 N_D) conditions, voltage

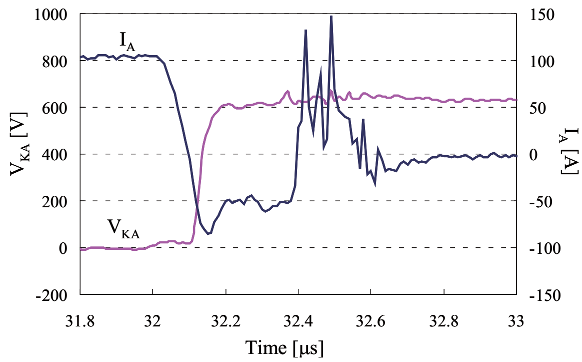

Fig. 4 Measured reverse recovery characteristics of Sample B (high carbon concentration).

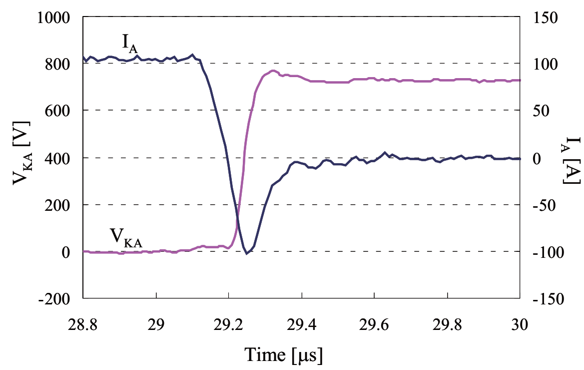

Fig. 5 Measured reverse recovery characteristics of Sample A (low carbon concentration).

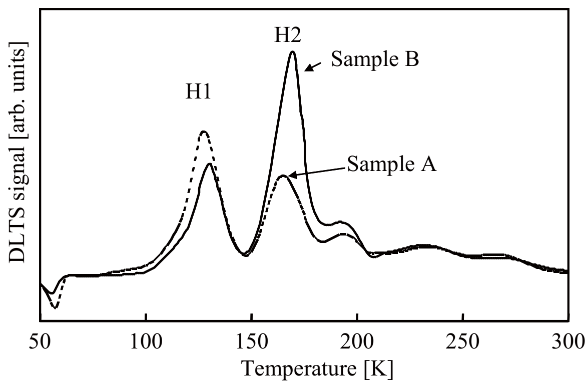

Fig. 6 Measured DLTS spectra for hole traps in samples A and B.

clumping was observed and a significant voltage change was also observed following voltage clumping. The simulated voltage waveform behavior is similar to the experimental results for sample B (high carbon concentration), as shown in Fig. 4. Therefore, it is predicted that a hole-trap at $E_T = E_V + 0.35$ eV has a substantial effect on the occurrence of dynamic avalanche phenomena, which is highly dependent on hole-trap concentration.

In order to examine the relationship between the hole-trap at $E_T = E_V + 0.35$ eV and defect complexes related to carbon impurities in silicon, cathode luminescence (CL) were selected as evaluation methods that are capable of detailed investigation of energy levels and defect complex identification. **Figure 8** shows CL spectra for samples A and B.[37] According to previous CL spectral studies, the C-line has been identified as a defect complex (C_iO_i) formed by interstitial carbon (C_i) and interstitial oxygen (O_i), and the G-line has been identified as a defect complex (C_iC_s) formed by an interstitial carbon (C_i) and substitutional carbon (C_s).[38-42] The peak heights are reported to be qualitatively proportional to defect complex concentrations and carbon impurity concentrations.[41,42] For both peaks, the C-line energy is equivalent to the energy of the hole-trap at $E_T = E_V + 0.35$ eV, and the peak intensity of sample B was higher than that of sample A, which strongly suggests that the root cause of the dynamic avalanche phenomenon is related to the C_iO_i complex. The energetically stable structure and energy states of the C_iO_i complex were also investigated using first-principle calculations based on density functional theory (DFT). As a result, the calculated structure of C_iO_i was similar to that previously reported,[43] and while evaluating the energy state it was possible to observe the energy level in the bandgap. **Figure 9** shows the obtained C_iO_i structure with an isosurface of ground state electron density related to the energy level introduced into the bandgap. It is noted that the electron density was located around C_i, so that carbon plays the role of introducing the energy level into the bandgap. It has been reported that C_iO_i complex formation by irradiation processes follows the following reaction mechanism:

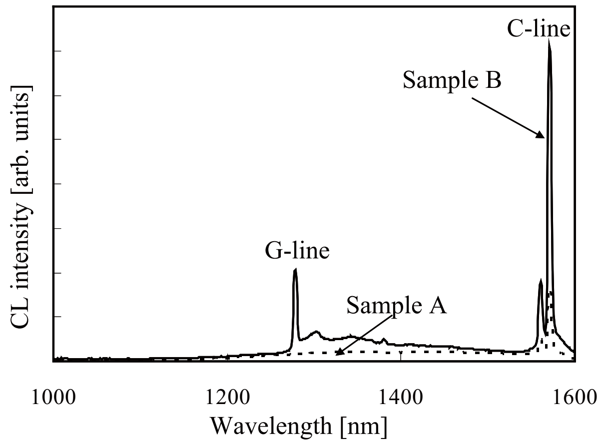

Fig. 8 Measured CL spectra for samples A and B.

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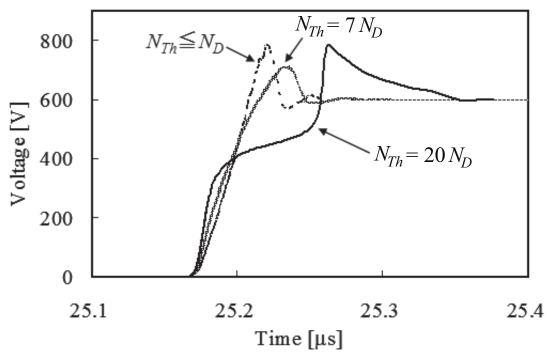

Fig. 7 Simulated voltage waveforms during reverse recovery (N_D: initial donor concentration, N_{Th}: hole trap concentration).

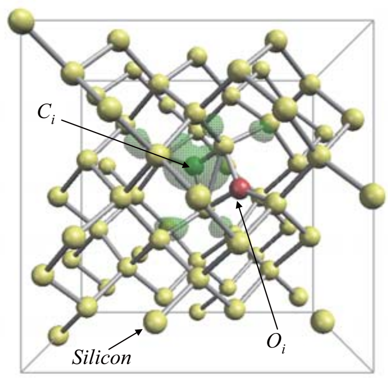

Fig. 9 Calculated structure for stable C_iO_i in silicon crystal with an isosurface of ground state electron density related to an energy level introduced into the bandgap.

$$Si_s \rightarrow Si_i , \qquad (6)$$

$$Si_i + C_s \rightarrow C_i , \qquad (7)$$

$$C_i + O_i \rightarrow C_iO_i , \qquad (8)$$

where Si_s is substitutional silicon, Si_i is interstitial silicon, and O_i is interstitial oxygen. From these reaction mechanisms, it is noted that C_iO_i is formed from carbon as the origin, and in the placement of carbon, C_s is replaced by C_i. Thus, C_s was also evaluated using first-principle calculations based on DFT and no introduced energy levels in the bandgap were observed, which indicates that C_s is electrically non-active. Therefore, carbon impurities are not able to act as hole-traps until the silicon crystal is irradiated. A series of these results indicates that control of the carbon impurity concentration is very important for helium-irradiated silicon PIN diodes and for control of electrical dynamic characteristics such as dynamic avalanching.

4. Conclusions

Helium irradiation techniques have been effectively used for power devices in electrical power transforming systems. The effect of carbon impurities in helium-irradiated silicon on the electrical dynamic characteristics of PIN diodes is investigated with respect to the reliability of power devices and electrical power transforming systems. Under conditions of high carbon concentration in helium-irradiated silicon PIN-diodes, the dynamic avalanche phenomenon is observed during the reverse recovery transient and the high hole-trap concentration at $E_T = E_V + 0.35$ eV was confirmed by DLTS measurement. Device simulations were performed taking into account the SRH model under similar experimental conditions, and the dynamic avalanche phenomenon is predicted due to the influence of the hole-trap at $E_T = E_V + 0.35$ eV. During the reverse-recovery period of increasing voltage, a hole-trap at $E_T = E_V + 0.35$ eV would act as a temporarily positive charge that leads to high effective electric fields due to an increase in the effective donor concentration. CL measurements revealed that a hole-trap at $E_T = E_V + 0.35$ eV is related to the C_iO_i complex, which implies that carbon plays a role in the introduction of the energy level into the bandgap, as revealed by DFT-based first-principle calculations. C_iO_i formation through irradiation processes originates in C_s. A series of these results suggests the mechanism of influence by which carbon impacts on the dynamic avalanche phenomenon, and reveals that control of the carbon impurity concentration in helium-irradiated silicon PIN diodes is very important for control of the electrical dynamic characteristics.

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- The Institute of Electrical Engineers of Japan
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