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Effect of $Z_{1/2}$, EH5, and Ci1 Deep Defects on the Performance of n-type 4H-SiC Epitaxial Layers Schottky Detectors: Alpha Spectroscopy and Deep Level Transient Spectroscopy Studies

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Meet The New Deputy Editors

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Effect of $Z_{1/2}$, EH_5 , and $Ci1$ deep defects on the performance of n-type 4H-SiC epitaxial layers Schottky detectors: Alpha spectroscopy and deep level transient spectroscopy studies

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Spectroscopic performance of Schottky barrier alpha particle detectors fabricated on 50 μm thick n-type 4H-SiC epitaxial layers containing $Z_{1/2}$, EH_5 , and $Ci1$ deep levels were investigated. The device performance was evaluated on the basis of junction current/capacitance characterization and alpha pulse-height spectroscopy. Capacitance mode deep level transient spectroscopy revealed the presence of the above-mentioned deep levels along with two shallow level defects related to titanium impurities ($Ti(h)$ and $Ti(c)$) and an unidentified deep electron trap located at 2.4 eV below the conduction band minimum, which is being reported for the first time. The concentration of the lifetime killer $Z_{1/2}$ defects was found to be $1.7 \times 10^{13} \text{ cm}^{-3}$. The charge transport and collection efficiency results obtained from the alpha particle pulse-height spectroscopy were interpreted using a drift-diffusion charge transport model. Based on these investigations, the physics behind the correlation of the detector properties viz., energy resolution and charge collection efficiency, the junction properties like uniformity in barrier-height, leakage current, and effective doping concentration, and the presence of defects has been discussed in details. The studies also revealed that the dominating contribution to the charge collection efficiency was due to the diffusion of charge carriers generated in the neutral region of the detector. The 10 mm^2 large area detectors demonstrated an impressive energy resolution of 1.8% for 5486 keV alpha particles at an optimized operating reverse bias of 130 V. © 2014 AIP Publishing LLC. [<http://dx.doi.org/10.1063/1.4883317>]

I. INTRODUCTION

Silicon carbide (SiC) is a promising semiconductor material due to its wide bandgap, and high thermal conductivity, breakdown electrical field, saturation electron drift velocity, radiation resistance, and excellent physical and chemical stability.^{1–6} Availability of detector grade single crystalline bulk SiC is limited by the existing crystal growth techniques that introduce macroscopic as well as microscopic crystallographic defects during the growth process.⁷ Recently, SiC based high resolution semiconductor detectors for ionizing radiations have attracted attention due to the availability of high-resistive, highly crystalline epitaxial layers with extremely low micropipe defect content ($<1 \text{ cm}^{-2}$). SiC Schottky detectors on epitaxial layers can be operated with a high signal-to-noise ratio even above the room temperature due to its high bandgap (low leakage current).^{8–10} However, intrinsic defects and impurity related complexes have been reported in as-grown SiC epilayers as well.^{11,12} Many of these defects are electrically active and can lead to increased detector leakage current and poor carrier lifetime and mobility by acting as trap or recombination/generation centers. The electrically active defects may lead to charge loss or detector output pulse with large rise times leading to incomplete charge collection. Therefore, it is very important to identify the electrically active defects in the epilayer and evaluate their role in affecting the ultimate detector

performance. Deep level transient spectroscopy (DLTS) is a very sensitive technique for the identification of defect related parameters such as energy level, concentration, capture cross-section, and spatial profile in semiconductors.¹³ A C-DLTS spectrum is generated from the temperature dependent capacitance transients followed by a saturated trap filling pulse applied to a semiconductor junction. The defect concentration, capture cross-sections, and the activation energy can then be extracted by analyzing the capacitance transients.

In this work, we have characterized Schottky barrier detectors fabricated on 50 μm thick 4H-SiC epitaxial layers. The detector performances were evaluated in terms of junction properties, leakage current, charge collection efficiency, and energy resolution using alpha pulse height spectroscopy. The performances of the detectors were found to be limited by the presence of point defects in the epitaxial layers. Hence C-DLTS measurements were carried out in these epilayer detectors in a wide range of temperature (80–800 K) to investigate the existing defects. Six distinct DLTS peaks were observed corresponding to six different trap centers. The defect centers were identified and characterized in terms of activation energies, trap concentrations, and capture cross-sections. One of the detected defects, located at $E_c - 2.4 \text{ eV}$, has been observed for the first time in 4H-SiC epitaxial layers.

II. EXPERIMENTAL PROCEDURE

A. Detector fabrication

The n-type epilayers were grown on $10 \times 10 \text{ mm}^2$ 4H-SiC (0001) substrates (n-type), which were highly doped

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with nitrogen and were off-cut 8° towards the $[11\bar{2}0]$ direction by a hot wall chemical vapor deposition (CVD) process using dichlorosilane (SiH_2Cl_2 , DCS) and propane (C_3H_8) as the precursors and hydrogen as the carrier gas. The Schottky barriers were formed on the epitaxial layers (Si face) by depositing thin (10 nm) circular Ni contacts (area $\sim 10 \text{ mm}^2$), which also act as the detector window. The thickness of the Ni contacts was so chosen that it has minimal alpha energy attenuation or scattering effect but is thick enough to obtain reliable electrical contacts as well. For the back contacts, 100 nm thick square ($\sim 40 \text{ mm}^2$) Ni contacts were deposited on the C face of the 4H-SiC substrates. A Quorum Q150T DC sputtering unit was used to deposit the metal contacts. A standard RCA cleaning of the samples was done prior to all contact depositions. The details of the detector structure can be found elsewhere.¹⁴

B. Detector characterization

The Schottky diodes were characterized for the junction properties through current-voltage (I-V) and the capacitance-voltage (C-V) measurements. The room temperature I-V characteristics of the samples were measured using a Keithley 237 high voltage source measure unit. The C-V measurements were carried out at a frequency of 1 MHz and the doping concentrations and the built-in potentials were calculated from $1/C^2$ -V plots.

To acquire the alpha pulse height spectra, an Amptek A250CF preamplifier was used first to obtain charge pulses from the detector irradiated with a standard $0.1 \mu\text{Ci } ^{241}\text{Am}$ source. The preamplifier charge pulses were fed to an Ortec 572 spectroscopy amplifier. A Canberra Multiport II ADC-MCA unit was used to generate the pulse-height spectra. To minimize the influence of any other electric field, the detector was kept inside a metal box, which was also being continuously evacuated to minimize scattering of the alpha particles by the air molecules. The energy calibration of the detection system was carried out using a precision pulser. The energy resolution values of the detectors were expressed in terms of full width at half maxima (FWHM) of the relevant peaks under investigation.

C. Defect characterization

For defect characterization, a SULA DDS-12 DLTS system is used in a capacitance mode. The DLTS system comprised of a pulse generator, a capacitance meter, a correlator module, and a PC based data acquisition and analysis software. The correlator module uses a modified double boxcar signal averaging algorithm. It automatically removes DC background from the capacitance signals and measures the capacitance transient in a given rate window. The correlator unit is capable of assigning four simultaneous rate windows in a single thermal scan. For sample temperature variation, the detectors were mounted in a Janis VPF 800 LN2 cryostat controlled by a Lakeshore LS335 temperature controller. Temperature scans ranging from 80–800 K were selected for a single run at a heating rate of 0.05 K s^{-1} .

III. RESULTS AND DISCUSSIONS

A. Electrical characterization

The forward bias characteristics in a $50 \mu\text{m}$ 4H-SiC epitaxial Schottky barrier detector are shown in Figure 1. The current-voltage characteristics of a Schottky barrier diode can be expressed by the Bethe's thermionic emission theory¹⁵ as given below

$$I = AA^*T^2 \exp(-\beta\phi_B) \left[\exp\left\{ \frac{\beta(V - IR_s)}{n} \right\} - 1 \right], \quad (1)$$

where A is the geometric area of the Schottky contact, A^* is the effective Richardson's constant ($146 \text{ A cm}^{-2} \text{ K}^{-2}$ for 4H-SiC), ϕ_B is the Schottky barrier height, n is the diode ideality factor, V is the applied bias, R_s is the series resistance, $\beta = \frac{q}{k_B T}$, where q is the electronic charge, k_B is the Boltzmann constant, and T is the absolute temperature. From the forward I-V characteristics and using Eq. (1), the ideality factor was calculated to be 1.2, which suggests the presence of a spatial non-uniformity in barrier-height distribution over the metal contact area. The barrier height for the Ni/4H-SiC contact was calculated to be 0.95 eV, using Eq. (1) and the forward characteristics. The reverse bias characteristic of the detector is also shown in Figure 1. The leakage current was found to be $\sim 9 \text{ nA}$ at a reverse bias voltage of -150 V .

Figure 2 shows the $1/C^2$ vs V plot obtained for the Schottky barrier detector. The inset shows the actual C-V plot. The effective doping concentration (N_{eff}) was calculated to be $1.98 \times 10^{15} \text{ cm}^{-3}$ and the built-in V_{bi} potential of the contact was found to be 1.5 V from $1/C^2$ vs V plots. The Schottky barrier height was also calculated from the C-V characteristics. Considering the standard band diagram for an abrupt p-n junction, the barrier height can be expressed as

$$\phi_{B(C-V)} = V_{bi} + V_n, \quad (2)$$

where V_n is the energy difference between the Fermi level and the conduction band minimum and can be expressed as

$$V_n = kT \ln \frac{N_C}{N_{\text{eff}}}, \quad (3)$$

FIG. 1. Variation of junction current as a function of applied bias for a $50 \mu\text{m}$ n-type Ni/4H-SiC epitaxial Schottky barrier detector.

FIG. 2. $1/C^2$ vs reverse bias plot for a $50\ \mu\text{m}$ n-type Ni/4H-SiC epitaxial Schottky barrier detector. The open circles are the experimental data points and the solid line is a straight line fit to the experimental data. Inset shows the original C-V plot.

where N_C is the effective density of states in the conduction band of 4H-SiC and is taken equal to $1.7 \times 10^{19}\ \text{cm}^{-3}$.¹⁶ The barrier height, thus, calculated from C-V measurements was 1.7 eV, which is higher than that obtained from the forward I-V characteristics. The difference between the two barrier height values can be explained as follows. Barrier height obtained from the forward I-V characteristics is generally dominated by current flow through the low Schottky barrier height locations over the entire metal contact area in an inhomogeneous Schottky diode, which results in lower surface barrier height. C-V characteristics, on the other hand, give an average value of the barrier height for the whole diode area.^{17,18} The larger value of barrier height calculated from the C-V measurements reconfirms the spatial inhomogeneity of the surface barrier height as was also inferred from the ideality factor value. The junction properties, especially the leakage current, are controlled by the presence of electrically active defects in the detector active volume, which, in turn,

FIG. 3. Variation of experimentally obtained ($\square$) and theoretically calculated ($\circ$) charge collection efficiency as a function of reverse bias voltage. The theoretically calculated separate contributions to the total CCE from charge drifts in depletion region (Δ) and from hole diffusion in neutral region (∇) are also shown. The solid line shows the variation in depletion width with reverse bias. The dotted line indicates the projected range of the 5486 keV alpha particles in 4H-SiC ($\sim 18\ \mu\text{m}$).

defines the detector performance. The defects affect the detector performance to various degrees depending on the defect parameters such as location in the band gap, concentration, and charge state. Thus, detectors fabricated on otherwise similar wafers can perform in a substantially different manner depending on the defect types and parameters.

B. Alpha pulse height spectroscopy measurements

The detector readily showed an alpha peak with charge collection efficiency (CCE) of $\sim 17\%$ at 0 V applied bias when exposed to a ^{241}Am source, suggesting a substantial diffusion of minority carriers. As can be seen from Fig. 3, the charge collection efficiency was observed to improve with increase in operating bias. Figure 3 also shows the separate contribution of charge carrier diffusion ($CCE_{\text{diffusion}}$) and drifting ($CCE_{\text{depletion}}$), towards the total observed CCE as a function of reverse bias. The CCE contributions were calculated using a drift-diffusion model as expressed below.¹⁹

$$\begin{aligned} CCE_{\text{theory}} &= \frac{1}{E_p} \int_0^d \left(\frac{dE}{dx} \right) dx \\ &+ \frac{1}{E_p} \int_d^{x_r} \left[\left(\frac{dE}{dx} \right) \times \exp \left\{ -\frac{(x-d)}{L_d} \right\} \right] dx, \\ &= CCE_{\text{depletion}} + CCE_{\text{diffusion}}, \end{aligned} \quad (4)$$

where E_p is the energy of the incident alpha particles, d is the depletion width at a given bias, dE/dx is the rate of loss of energy of the implanted alpha particles as they penetrate the 4H-SiC epilayer and obtained from the Bragg curve plotted using SRIM 2013,²⁰ x_r is the projected range of the alpha particles incident with energy E_p and L_d is the diffusion length of the minority carriers. From Fig. 3, it could be seen that the experimentally observed CCE values reached a maximum value of ~ 0.87 at an applied bias of 130 V and started to decrease slowly thereafter. A saturated CCE value less than 1 suggests that a fraction of the generated charge carriers is getting trapped and eventually lost (recombine) in the defect centers. It can also be noticed from Figure 3 that the major contribution towards the observed CCE was from the diffusion of the charge carriers (more than 50%). The contribution of the drifting of charge carriers ($CCE_{\text{depletion}}$) towards the CCE was seen to increase steadily with the reverse bias and becomes almost equal to $CCE_{\text{diffusion}}$ at higher bias voltages. The reason behind the dominating contribution of charge carrier diffusion towards the CCE is because of the fact that the depletion width at the highest applied bias ($\sim 10\ \mu\text{m}$) was still much less compared to the penetration depth of the 5486 keV alpha particles ($\sim 18\ \mu\text{m}$) in 4H-SiC and hence a substantial part of the charge carrier generation takes place in the neutral region of the detector. However, for a superior detector performance, the generation of charge carriers is preferred to occur in the depletion region in order to obtain optimized charge transport properties. The reverse bias was further increased to widen the depletion width so that the contribution of charge carrier drifting to the CCE could increase. However, further increase in bias voltage led to increased leakage currents, which deteriorated the detector

performance. The depletion width (d) of a Schottky junction of a given material and, at a given bias, depends on the effective doping concentration of the semiconductor material as shown in Eq. (5). Electrically active defects can behave as acceptor or donor levels, thus, controlling the effective doping concentration and hence the depletion width

$$d = \sqrt{\frac{2\epsilon\epsilon_r(\phi_B - V)}{qN_{eff}}}. \quad (5)$$

The dependence of detector energy resolution with the reverse bias is shown in Figure 4. The percentage energy resolution improved with the reverse bias because of improved charge collection and lowering of detector capacitance (reduction of series noise). However, the resolution was seen to deteriorate with further increase in reverse bias due to increase in leakage current as was evident from the increase in the corresponding pulser peak width shown along-with in Figure 4. Also, increase in the depletion width leads to inclusion of more number of defects within the detector active volume leading to poor performance of the detectors. Figure 5 shows the best pulse height spectrum obtained with the optimized bias settings with an energy resolution of 1.8% for the 5486 keV alpha particles.

From the discussions above and in Sec. III A, it follows how substantially the presence of defects in the semiconductors could affect the detector performance by altering the leakage current, effective doping concentration, active volume, and charge collection efficiency. Hence, it was decided to characterize the defects present in these epitaxial layers. Section III C deals with an in-depth discussion of the defect detection and identification in a 4H-SiC epitaxial layer detector used in the present study.

C. DLTS analysis

The DLTS measurements were carried out in a temperature range of 80–800 K with a steady-state reverse bias of -2 V. The pulsing was done to 0 V from the steady-state

FIG. 4. Variation of detector energy resolution as a function of reverse bias voltage. The variation of the peak width (FWHM) of the pulser recorded simultaneously has also been plotted.

FIG. 5. A ^{241}Am pulse height spectrum obtained using the $50\text{ }\mu\text{m}$ n-type Ni/4H-SiC epitaxial Schottky barrier detector reverse biased at 130 V.

reverse bias to fill/populate the majority carrier traps present within the steady state depletion width. A pulse width of 1 ms was chosen in order to ensure saturation trap filling. In a capacitance DLTS mode, the system relaxes into equilibrium by thermally emitting the trapped charges after the termination of the filling pulse resulting in capacitance transients. The thermally activated emission rate e_n can be expressed as below

$$e_n = (\sigma_n V_{th} N_C / g) \exp(-\Delta E / kT), \quad (6)$$

where σ_n is the carrier capture cross section, $\langle V_{th} \rangle$ is the mean thermal velocity, N_C is the effective density of states, g is the degeneracy of the trap level and was considered to be equal to 1 in the present calculations, and ΔE is the energy separation between the trap level and the carrier band. The emission rate is related to the capacitance transient by the following relationship:

$$C(t) = C_0 + \Delta C \exp(-te_n), \quad (7)$$

where C_0 is the junction capacitance at steady-state reverse bias voltage, ΔC is the difference in capacitance change measured within the rate window. The trap concentration N_t was calculated using the following expression:

$$N_t = 2 \left(\frac{\Delta C(0)}{C} \right) N_{eff}, \quad (8)$$

where $\Delta C(0)$ is the difference in capacitance change between the two edges of the filling pulse. The rate windows were defined by an initial delay, which is actually a delay set for the emission rate calculations following the termination of the filling pulse. The initial delay is related to the rate window τ as follows:

$$\text{Initial delay (ms)} = \frac{1}{(4.3 \times \tau)}. \quad (9)$$

Figures 6(a) and 6(b) show representative DLTS spectra in the temperature range of 80 to 140 K using a smaller set of initial delays and 80 to 800 K using a larger set of initial

FIG. 6. DLTS spectra obtained using the 50 μm n-type Ni/4H-SiC epitaxial Schottky barrier detector in a temperature range (a) 80–140 K with the smallest initial delay, (b) 80–800 K with the largest initial delay.

delays, respectively. The peaks appeared at different temperatures corresponding to different defect levels. In total, six distinct peaks were observed in the entire temperature scan range of 80–800 K and are numbered as Peaks #1 to #6. The negative peaks indicate that the detected traps are majority carrier traps (electron traps in this case). The activation energy is calculated from the Arrhenius plots (T^2/e_n vs $1000/T$). Figure 7 shows the Arrhenius plot for all the peaks obtained from the DLTS scans. The defect parameters were extracted from the DLTS scans using the equations described above and is summarized in Table I.

The trap levels corresponding to Peak #1 and Peak #2 were found to be located at $E_c - 0.13$ eV and $E_c - 0.17$,

FIG. 7. Arrhenius plots obtained for the Peaks #1 - #6 corresponding to the DLTS spectra shown in Figure 6.

TABLE I. Defect parameters obtained from the DLTS measurements.

Peak #	$\sigma_n \text{ cm}^2$	$\Delta E \text{ eV}$	$N_t \text{ cm}^{-3}$	Possible trap identity
Peak 1	4.13×10^{-15}	$E_c - 0.13$	1.3×10^{13}	Ti(h) ^a
Peak 2	2.50×10^{-15}	$E_c - 0.17$	3.6×10^{13}	Ti(c) ^a
Peak 3	3.36×10^{-15}	$E_c - 0.67$	1.7×10^{13}	$Z_{1/2}$ ^b
Peak 4	3.73×10^{-15}	$E_c - 1.04$	2.1×10^{13}	EH ₅ ^c
Peak 5	3.22×10^{-17}	$E_c - 1.30$	7.9×10^{12}	Ci1 ^d
Peak 6	1.53×10^{-11}	$E_c - 2.40$	5.6×10^{12}	Unidentified

^aReferences 21–25.

^bReferences 23, 26–36.

^cReferences 31 and 37, and 38.

^dReference 37.

respectively, where E_c is the conduction band minimum. Both the defect levels have been identified as titanium substitutional impurity. Dalibor *et al.*^{21,22} have reported two similar defect levels located at $E_c - (0.117 \pm 0.008)$ eV and $E_c - (0.160 \pm 0.010)$ eV from DLTS studies of Ti⁺ implanted 4H-SiC, which they attributed to the ionized titanium acceptor Ti³⁺ ($3d^1$) residing at hexagonal and cubic Si lattice sites, respectively. Gelczuk *et al.*²³ also reported similar trap levels and assigned them to the Ti impurities at hexagonal and cubic Si lattice sites. Zhang *et al.*²⁴ also assigned a defect level located at $E_c - 0.16$ eV to a Ti electron trap level. Castaldini *et al.*²⁵ assigned a trap level located at $E_c - 0.17$ to chromium or titanium impurities (acceptor like) in hexagonal position. The trap center related to Peak #3 was found to be located at 0.67 eV below the conduction band edge. Several groups have reported the presence of a similar defect level often designated as $Z_{1/2}$.^{26–30} However, the exact microscopic structure is still unknown and several theories exist in the literature regarding the probable structure of $Z_{1/2}$ centers. As summarized by Zhang *et al.*,²⁴ $Z_{1/2}$ is most likely related to defect complexes involving equal number of carbon and silicon sites. The possible structures listed by them, obtained from the existing literatures^{26,31,32} are silicon and carbon vacancy complexes ($V_{\text{Si}} + V_{\text{C}}$), antisite complexes ($\text{Si}_{\text{C}} + \text{C}_{\text{Si}}$) pairs, or a pair of an antisite and a vacancy of different atoms. However, their own findings were more inclined towards a divacancy like structure of the $Z_{1/2}$ defect. Eberlein *et al.*,³³ on the other hand, reported that the participation of carbon interstitial with nitrogen can also form defect levels with similar activation energy. $Z_{1/2}$ center is also reported to be responsible for the reduction of carrier lifetime by several authors.^{23,34–36} The activation energy corresponding to peak #4 was found to be located at 1.04 eV below the conduction band edge. A defect level reported by Alfieri *et al.*,³⁷ located at $E_c - 1.03$ eV and designated as EH₅, is the closest match with the Peak #4 observed in our case. Beyer *et al.* has also detected similar defect level ($E_c - 1.07$ eV) in 2.5 MeV electron irradiated 4H-SiC.³⁸ EH₅ defect has been found in ion irradiated 4H-SiC and has been attributed to a carbon cluster.³¹ The activation energy of Peak #5 was found to be 1.30 eV. Alfieri *et al.*³⁷ reported a similar defect center Ci1 in a chlorine implanted n-type 4H-SiC epitaxial layer. The Peak #6 was found to have the highest activation energy (2.40 eV) among all the defect centers observed in the DLTS scans and remains unidentified as

the corresponding activation energy does not match with any known defect level in 4H-SiC that has been reported in the literature. The trap concentrations corresponding to Peaks #1–#4 were all of the order of 10^{13} cm^{-3} with the Ti impurity (cubic Si site) being the maximum. Peaks #5 and #6 were found to be one order of magnitude less in concentration.

IV. CONCLUSION

In an attempt to fabricate alpha detectors with a large active volume, we used $50 \mu\text{m}$ thick 4H-SiC epitaxial layers as detector material. However, based on the electrical characterization and alpha spectroscopic measurements, the device performance was found to be limited by the presence of various point defects within the active volume of the detector. The detectors were investigated for defects using deep level transient measurements and six different defect centers were detected in a temperature scan range of 80–800 K. Substitutional titanium impurities in Si sites were found to be among the shallow levels. $\text{Z}_{1/2}$, EH_5 , and Ci1 were among the deep levels present with concentrations of the order of 10^{13} cm^{-3} . A new deep lying defect level located at $E_c - 2.4 \text{ eV}$ was also observed, which has not been reported till date.

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