



Interface improvement of epitaxial 4H-SiC based Schottky diodes by selective heavy ion irradiation

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Abstract

This work reports selective high-energy heavy ions irradiation for improving the interfacial properties of epitaxial SiC-based Schottky barrier diode (SBD). Ni/4H-nSiC(0001) SBDs have been fabricated and irradiated using 200 MeV silver ions at a fluence of 1×10^{12} ions/cm² in selective and in blanket ways under same experimental conditions. Electrical performance of the blanket way-irradiated SBD was found almost destroyed. In stark contrast, barrier height is enhanced from 1.16 eV to 1.41 eV and ideality factor reduced from 1.81 to 1.76 in selectively irradiated SBD. Moreover, interface trap/defect states density has been reduced from 1.56×10^{13} eV⁻¹ cm⁻² to 6.47×10^{12} eV⁻¹ cm⁻² after selective irradiation of SBD. Role of heavy ions irradiation-induced electronic excitations in refinement of atomic-scale interfacial defects/disorders of the SBD and, hence, modification in its electrical performance has been discussed. Photoluminescence studies are also performed to get insight into the measured device performance.

Keywords Defects · Swift heavy ion irradiation · Interface states · SiC · Schottky barrier diode

Introduction

The comfort and transportation of the modern society is dependent on the generation and distribution of the power. It is only possible through enhancement in the performance of the power devices (Baliga 2005). Silicon (Si)-based power devices were of prime choice for several decades owing to their high manufacturing capability and lower cost. Unfortunately, Si has approached its theoretical limits and implementation of wide bandgap semiconductors such as SiC, GaN, diamond, Ga₂O₃, etc. has been emerged as an alternative. Contrast with its counterparts, SiC is a preferred material for power devices due to maturity in its crystal quality

and availability in the market (Dimarino et al. 2015; Tsao et al. 2018).

The most fundamental and mature case of a power devices are Schottky barrier diodes (SBDs). Precisely, control over interface properties is a crucial factor for enhancing its performance (Baliga 2005; Kumar et al. 2012; Omar et al. 2014). Presence of electrically active defects at the interface, and in the bulk of the material deteriorate the performance, reliability, and stability of the SBDs. Interface- and bulk-level defects cause a reduction in the barrier height and increment in the leakage current in SBDs. For these reasons, their full potential for adoption in high-power, high-frequency switching, and many other applications is hindered (Omar et al. 2014; Kumar et al. 2016; Kumar et al. 2015; Kumar et al. 2014; Singh 2006; Kumar et al. 2020). Compelling factors for the creation of defects in the SBDs include; structural imperfections, contaminations, unsaturated bonds, damages caused by metal deposition, formation of residual native oxide, etc., in the semiconductors (Kang et al. 2017; Gulen et al. 2011; Gammon et al. 2013).

Swift heavy ions (SHI) irradiation has been proven to be a versatile technique to advance the semiconductor technology (Wesch and Wendler 2016). For example, literature reported that SHI irradiation (1) is efficacious in the generation of new phases especially silicides at the

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metal–silicon interface, and (2) found adequate in tailoring the lifetime of minority carriers in semiconductor devices. Moreover, synthesis and modification of nanostructured materials for advance device applications is also feasible with SHI irradiation (Avasthi and Mehta 2011). Recently, selective swift heavy ion irradiation is used to remove the atomic-level defects from the crystalline semiconductor. Silicon was selectively irradiated with swift heavy ions and atomic-level disorders/defects, from surface and bulk of the material, were found swept out from the irradiated site. The swept defects found accumulated at the boundary of the irradiated and masked region (Sen and Akhtar 2002; Sen et al. 2000). Using this technique, the electrical properties of Si-based p–n junction were enhanced by modifying their interface and bulk structures (Kumar et al. 2013). Moreover, the performance of SiC-based SBDs, i.e., barrier height and leakage current, have been significantly improved using same methodology (Kumar et al. 2020; Kumar et al. 2018; Kumar and Maan 2018). A deep understanding of such improvement demands further studies on interface and bulk-level refinement in the selectively irradiated devices.

Behavior of interface of the SBDs can be understood in terms of SHI irradiation-induced modifications in the localized electronic energy states (so-called interface trap states) present at its interface. It is because, the modifications of interface trap states will amend the current transportation mechanism across the interface of SBDs and hence their performance (Baranwal et al. 2009; Spicer et al. 1980). Therefore, evaluation of interface trap states density and their distribution is highly desired and it will be highly impactful from both technological and physics point of view. Additionally, SHI irradiation produces defects in the material at the end of their range, i.e., in the nuclear energy loss regime (Sen and Akhtar 2002; Sen et al. 2000; Madito et al. 2019; Tunhuma et al. 2019). A fundamental understanding of such produced defects is the first step to rationalize the performance of the SiC based SBDs. These investigations will be helpful in comprehending the implications of selective heavy ion irradiation in future microelectronic devices.

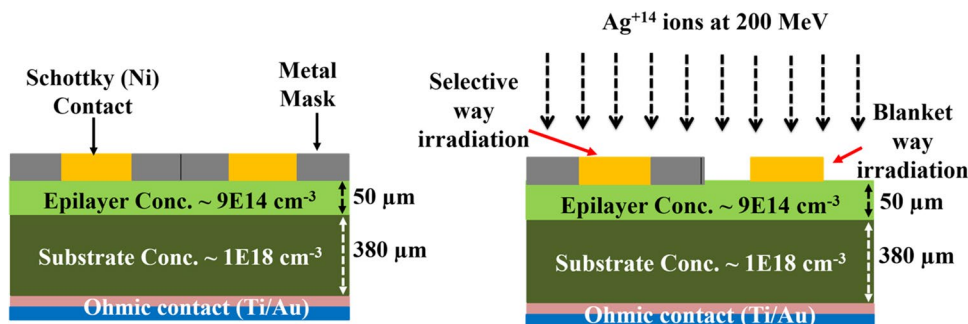
Therefore, the aim of the present work is to investigate the interface and bulk of the selectively heavy ion-irradiated SiC-based SBD. Interface of the devices has been probed with capacitance-based method; whereas a non-destructive technique, i.e., Photoluminescence (PL) spectroscopy, is implemented to characterize the bulk-level modifications in the SiC. Peaks in the measured PL spectra have been recognized and assigned with data from the literature. Contribution of nuclear and electronic energy transfer mechanisms has been discussed in detail to support the observed electrical behavior of the devices.

Experimental

For device fabrication, research grade nitrogen-doped n^+ 4H-SiC (0001) wafer of 50 μm thick epitaxial layer on 8° off-axis Si-face with concentration $\sim 1 \times 10^{15} \text{ cm}^{-3}$ was used. The wafer was thoroughly cleaned employing standard chemical procedure, i.e., degreasing, RCA-1, RCA-2, and Piranha. Molybdenum metal mask of thickness 0.1 mm was used to delineate the Schottky contacts and also for selectively irradiate the device. The choice of the metal sheet was based on its stiffness and microelectronic compatibility. The grooves in the metal sheet were made with a computer numerical control (CNC) wire cut electric discharge machine (EDM). The requirement of steep walled grooves comes from the need of fabricating notch-free Schottky contacts and selective irradiation of fabricated devices. After that, the fabricated metal masks were cleansed with HCl and deionized water. These metal masks were baked for 3 h at 120°C to eliminate any degassing phenomena while their usage in device fabrication. These metal masks were placed on the Si-face of the cleaned wafer using photoresist and then loaded into the e-beam metallization chamber. Nickel metal of thickness 200 nm was deposited on the Si-face of wafer using e-beam evaporation method and subsequently Schottky device of size 1.6 mm in diameter was fabricated. Ohmic contact was realized on the C-face of the wafer with dual layer metallization of Ti (300 \AA) and Au (2000 \AA) using e-beam evaporation system in vacuum range of 10^{-7} Torr. Thereafter, the device was vacuum annealed at 350°C in a chamber under the flow of Ar gas at 365 cc/min for 30 min (Wesch and Wendler 2016). Device was irradiated with Ag^{14+} ions at 200 MeV (maximum available energy at the facility) with a fluence of 1×10^{12} ions/ cm^2 employing 15 UD Pelletron accelerator facility at IUAC, New Delhi. Devices normally got damaged within the selected fluence range (Strelchuk et al. 2009). To generate a contrast with this understanding, the ion irradiation was carried out in two ways namely “blanket way” and “selective way”. In *blanket way*, masks were removed from the surface of the wafer and then device was irradiated. In other words, the device and its surrounding area were irradiated. On the other hand, in *selective way*, the mask was retained on the surface of the wafer and then device irradiated, i.e., the ions were bombarded only to the Schottky contact and blocked in its surrounding area. A schematic of the performed experiment is shown in Fig. 1. All devices were fabricated and irradiated under same run and other environmental conditions.

Keithley 4200 SCS was used for current–voltage (I–V) measurements and Agilent 4284 A was used for capacitance–voltage (C–V) measurements of the devices. The

Fig. 1 **a** Schematic of the fabricated devices (material specifications: CREE, USA); **b** ion irradiation on the device in selective way (left side, i.e., with metal mask surrounding the periphery of the device to block the ion’s beam) and in blanket way (right side, i.e., device including surrounding area irradiated with ions)



current–voltage (I–V) characteristics of the fabricated devices were acquired using Suss Microtek probe station. Devices were held on the vacuum connected gold plated chuck of the probe station.

Results and discussion

To get the forward bias characteristics, DC bias was swept from 0 to 2 V. The observed I–V and corresponding Ln (J)–V characteristics of the pristine and selectively irradiated diodes are shown in Fig. 2a, b, respectively.

The current flow in the moderately doped semiconductors-based SBD is predominately attributed to the majority charge carriers. The current–voltage characteristics of the forward-biased Schottky barrier diodes can be explained using thermionic-emission (TE) model as (Sharma 1984):

$$J = J_s \left[\exp \left(\frac{qV}{\eta kT} \right) - 1 \right], \tag{1}$$

where J_s is the saturation current density and can be given as:

$$J_s = A^* T^2 \exp \left(- \frac{q\phi_B}{kT} \right), \tag{2}$$

where ϕ_B is the zero bias barrier height, q is the electronic charge, k is the Boltzmann constant, T is the measuring

temperature, and A^* is the Richardson constant ($146 \text{ A/cm}^2\text{K}^2$) (Baliga 2005). Moreover, η in Eq. (1) is known as the ideality factor, and can be represented as:

$$\eta = \frac{q}{kT} \left(\frac{dV}{d \ln(J)} \right). \tag{3}$$

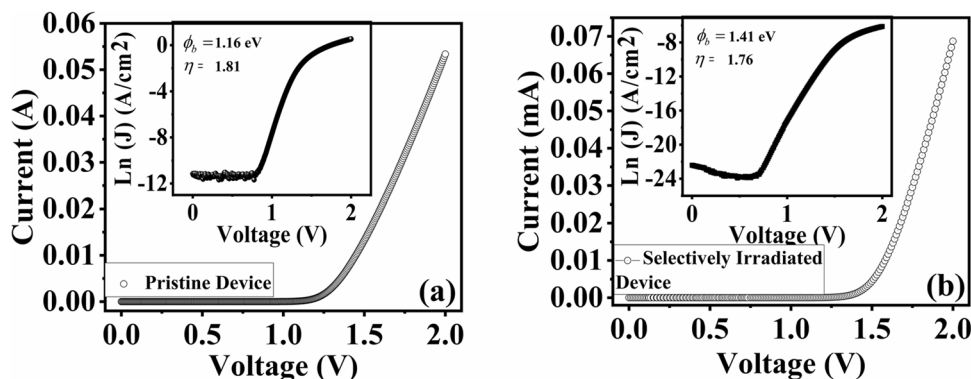
The intersection of straight line part of forward bias $\ln(J) - V$ plot at vertical axis determines the value of $\ln(J_s)$. Using $\ln(J_s)$ value, the zero bias barrier height can be determined as (Sharma 1984):

$$\phi_B = \frac{kT}{q} \ln \left(\frac{A^* T^2}{J_s} \right), \tag{4}$$

where all symbols have their usual meanings.

In present work, the I–V characteristics of the blanket way-irradiated device were found totally damaged (Kumar et al. 2020), and not shown here. This might be due to the formation of defects in the material in the nuclear energy loss regime of the irradiated ions. The formation of buried layer of defects and their complexes, at the end range of incoming ions, damaged the device under discussion (Kumar et al. 2020; Kumar et al. 2018). Therefore, in the foregoing discussion, pristine and selectively irradiated device would be the focus of this work. The barrier height and the ideality factor values for pristine and selectively irradiated devices were determined using Eqs. 3 and 4, which came out as 1.16 eV and 1.81, and 1.41 eV and 1.78, respectively.

Fig. 2 Current–voltage (I–V) and corresponding Ln (J)–V plots of the **a** Pristine and **b** selectively irradiated Schottky barrier diodes



The above calculated values of electrical parameters in forward bias reveal that the performances of the selectively irradiated device have been significantly improved. These findings attribute to the removal of defects from active area of the selectively irradiated SBD (Sen and Akhtar 2002; Kumar et al. 2018). To support the argument, interface state density has been calculated in the pristine and selectively irradiated devices using method proposed in Ref. (Chattopadhyay et al. 1998; Chattopadhyay 1996). This method is based on the forward bias capacitance measurements in the device, at low and high frequencies. Since interface states behave differently at low and high frequencies, the used method is extremely sensitive. The equation governing relationship between interface states and the capacitance is given as (Chattopadhyay et al. 1998):

$$D_{it} = \sqrt{\frac{q\epsilon_{Si}N_d}{2\psi_s} \frac{C_{LF} - C_{HF}}{qC_{HF}}}, \quad (5)$$

where C_{HF} and C_{LF} are capacitances at low (1 kHz) at high (1 MHz) frequencies, N_d is the effective doping concentration and other symbols have their usual meanings. Moreover, in Eq. (5), ψ_s is the surface potential which can be calculated using (Chattopadhyay et al. 1998):

$$I = A^*T^2 \exp\left(\frac{-q\psi_s}{kT}\right) \exp\left(\frac{-qv_n}{kT}\right), \quad (6)$$

where v_n is the distance between fermi level and conduction band and can be found as:

$$v_n = \frac{kT}{q} \ln\left(\frac{N_c}{N_d}\right). \quad (7)$$

Using Eq. (6), the values of surface potential w.r.t. applied bias is calculated and shown in Fig. 3.

It can be seen in Fig. 3a, b that ψ_s is decreasing linearly until reaching a critical voltage (V_C) beyond which effect the series resistance will be effective. The point $\psi_s(I_C, V_C)$ at which non-linearity in V_C commences represents the corresponding critical surface potential. It is worthy to note in Fig. 3a, b that critical surface potential value has been increased after selective ion irradiation, which is due to decrement in the surface states. Moreover, V_C has been decreased after selective ion irradiation which attributes to the defects production at the end of ions range as discussed in later sections.

Furthermore, Fig. 4a, b represents the measured C–V data at high (1 MHz) and low (1 kHz) frequencies for pristine and selectively irradiated devices.

It can be seen in Fig. 4a that the low frequency capacitance (C_{LF}) remains almost constant up to 1.0 V, then rising sharply and saturates at 2.0 V. The high frequency capacitance (C_{HF}) starts increasing slowly up to 1.25 V and then increasing sharply up to 2.0 V. However, in Fig. 4b, both C_{LF}

Fig. 3 The calculated values of surface potential in **a** pristine and **b** selectively irradiated device

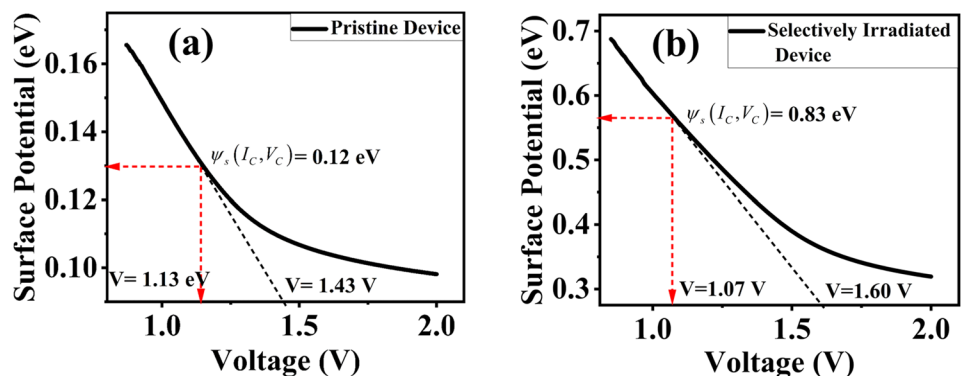
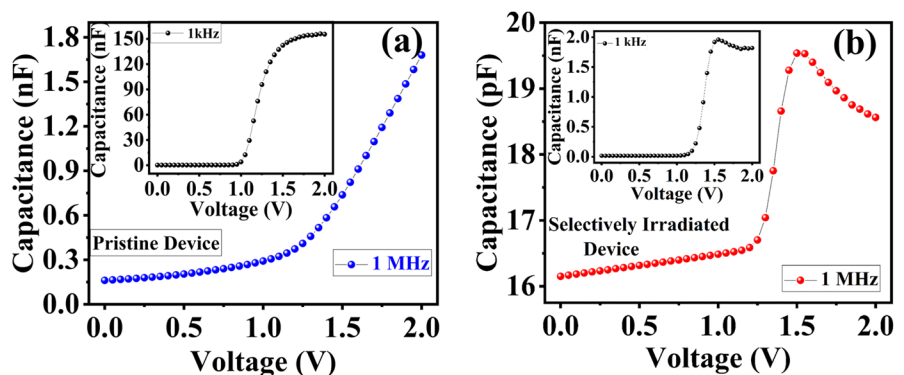


Fig. 4 Capacitance–voltage profiling of the **a** pristine and **b** selectively irradiated SBDs at high and low frequencies (shown in the inset)



and C_{HF} are first increasing slowly, then rising sharply and reached at maximum value at ~ 1.5 V and decreased after that. It is worth mentioning here that trends shown in Fig. 4a, b are a consequence of interface trap states present in the fabricated device (Kumar et al. 2016).

Using the maximum values of capacitance from these plots, the distribution of interface state density, D_{it} , within the energy gap of the SiC has been calculated for pristine and selectively irradiated devices and shown in Fig. 5a, b.

It can be seen in Fig. 5a that the density of interface trap states is decreasing as moving from edge of conduction band to the mid-gap of semiconductor. Selectively irradiated device is following the same trend as shown in Fig. 5b. However, a comparison of Fig. 5a, b reveals that the interface states density decreases by an order of magnitude after selective irradiation of the device. These results imply that removal of atomic-level defects from interface leads to improvement in barrier height of the selectively irradiated device as mentioned earlier. It is worth mentioning here that device under discussion was already vacuum annealed and selective irradiation further reduces D_{it} from $1.56 \times 10^{13} \text{ eV}^{-1} \text{ cm}^{-2}$ to $6.47 \times 10^{12} \text{ eV}^{-1} \text{ cm}^{-2}$ which is much higher than previously reported (Gupta et al. 2011). These findings emphasize that the selective heavy ion irradiation technique is an effective technique to improve the interface.

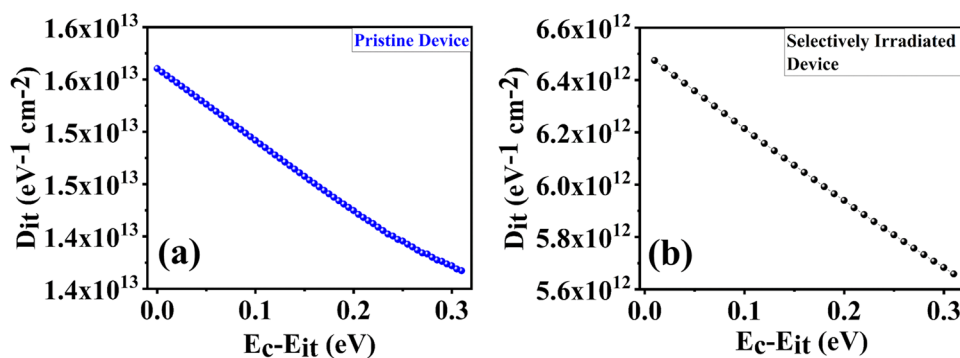
A possible mechanism underlying these improvements can be described in terms of swift heavy ion irradiation-induced electronic excitations in the material. Swift heavy ions deposit their energy in the form of ionization and separation of atoms of the target media. Due to this, a local electric field will be generated along the path of the incoming ions, which subsequently increase the kinetic energy (KE) of the atomic state of the material. This increased KE relaxed by its transfer to the nearby atoms in the form of electronic excitation. Moreover, electronic excitations cause large longitudinal movements of material atoms from their mean positions (Sen and Akhtar 2002; Sen et al. 2000). This large amplitude atomic motion introduced anharmonic forces in the Si and C atoms of the SiC material. As a result,

the vibrational frequency of the SiC atoms will be different from their optic and acoustical modes, which probably lies within the bandgap of SiC. Such vibrational modes of frequency are known as intrinsic localized modes (ILMs) or quodons. These quodons move from atoms to atoms without any sign of structural modification in the irradiated region of the target material (Sen and Akhtar 2002; Cuevasa et al. 2003). Moreover, ion-irradiation-induced non-linearity in the atomic forces of SiC is necessary for longer propagation of the quodons as they disperse in linear systems. These quodons moves defects from the irradiation site (i.e., the Schottky contact area) to masked area. Literature suggested that quodons are scattered by lattice disorders, which cause a change in momentum of the quodon. This change in momentum immediately imposes a pressure on the atomic-level defect and let those moves out from the source of quodons, namely, the ion track (Gupta et al. 2011). In this way, defects move away from the irradiated region in SiC. Moreover, at the boundary of the irradiated and masked region, these quodons will relax via localization of their energy and causes rearrangements of local atoms, i.e., under the metal mask. This rearrangement of atomic defects at the interface and bulk of SiC causes improvement in barrier height and ideality factor of the device.

Capacitance–voltage profile was used to calculate the effective doping concentration in the device. The effective doping concentration found to be decreased from 1.45×10^{15} to $7.03 \times 10^{14} \text{ cm}^{-3}$ after selective ion irradiation. This attributes to the defects produced in the material at the end range of the irradiated ions (Sen et al. 2000). Size as well as concentration of defects depends on the type and fluence of the projected ions, and on the doping level of the target material (Kalinina et al. 2014). The defects will capture free charge carrier and, hence, lowered the effective doping concentration in the material.

This reduction of effective carrier concentration results in the decrease in the built-in potential from 1.57 to 0.84 V after selective irradiation. The series resistance in device was also calculated using Cheung's method (Cheung and Cheung 1986), which found to be increased from 9.88 Ω

Fig. 5 Variation of interface states density with distance from conduction band edge in **a** pristine and **b** selectively irradiated SBDs



to 4.92 k Ω after selective ion irradiation. This is due to the fact that the epilayer of the used 4H-SiC was of 50 μm thick and the range of the projected ions (calculated using TRIM code in the present device structure) came as 15.65 μm . This implies that the projected ions are stopped in the active region of the device and produce defects at the end of their range. These defects result in the increase in the series resistance and decrease in the built-in potential of the device.

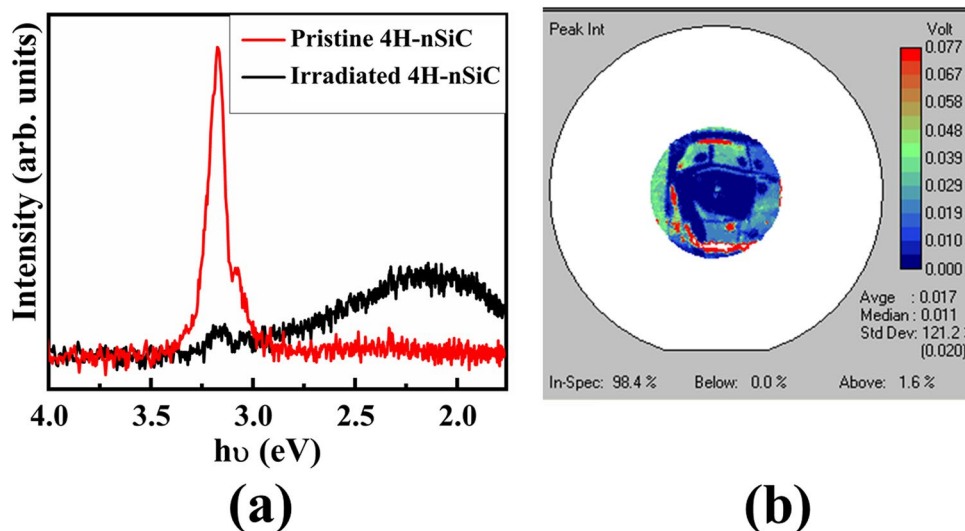
To get a deep insight into material's quality and irradiation-induced defects, photoluminescence studies are carried out and shown in Fig. 6a, b.

Figure 6a shows the PL spectra of pristine material which exhibit a strong peak, so called “zero phonon line (ZPL)”, in the near band edge region ($E_g = 3.24$ eV). This peak attributes to the recombination of exciton bound to neutral nitrogen at the cubic sites in the SiC (Ahoujja et al. 2004). Another peak is observed at 3.18 eV, which is caused by the neutral nitrogen bound exciton at the hexagonal site. High binding energy at cubic site leads to more localized exciton, which enhance the probability of its recombination without momentum-conserving photons. This can be justified by comparing the intensity of the cubic site and hexagonal site (Scott 1999). Another peak is found at 2.92 eV, which attributes to the nitrogen donor sites or a thermodynamically induced state associated with Shockley stacking faults (SSFs). The expanded SSFs can shrink by annealing at temperatures 500 K (Miao et al. 2001).

It can be seen in Fig. 6a, that intensity of the near band edge excitation has been reduced after ion irradiation. Peak fitting reveals that its position is shifted at 3.16 eV on the photon energy scale. Such findings reveal that some defects are formed in the material under discussion. These defects act as active recombination centers, whose energy position exist in the band gap of the SiC. Capturing of the free charge carriers by these defects results in the suppression of direct

electron–hole recombination. Therefore, lesser charge carriers (electron here) would emit back into the valence band and emit less energy in the form of light. Consequently, the intensity will be reduced as observed for irradiated samples in Fig. 6a. The value of the full width half maximum (FWHM) of the pristine and irradiated device was calculated to be 0.09341 nm and 0.2632 nm, respectively. The increased value of the FWHM and reduced intensity in photoluminescence spectra confirm that deep-level defects are formed in the irradiated SiC. Additionally, the defect band with a wide energy spectrum centred at 2.150 eV is also appeared in irradiated SiC, which mimic the reported literature (Kalinina et al. 2004). These findings imply that irradiation produces a wide range of defects having different energy levels in the material under reference. It is interesting to see that the defect level due to SSF, situated at 2.92 eV in the pristine material, has been quenched out after ion irradiation. It might be due to the ion irradiation-induced rise in temperature of the material. As stated earlier, these SSF have property to quench at moderate temperatures, and ion irradiation produces a very high temperature for short time duration in close proximity to the incoming ion. Therefore, it is believed here that ion irradiation is also very useful tool in healing of some stacking faults in the SiC. Moreover, photoluminescence mapping of the material under discussion is also carried out and shown in the Fig. 6b. It can be seen in Fig. 6b that the peak intensity in the pristine part has some finite value, while it is significantly reduced after irradiation. These results reconfirm that defects are formed in the bulk of the material. The overall changes in the material after ion irradiation can be explained on the basis of energy loss mechanisms of incoming ions in host material. It is well known that ions lose their energy via electronic and nuclear energy loss mechanisms during their wake through matter. In the starting range of ions, where electronic energy loss

Fig. 6 **a** Photoluminescence spectra of the pristine and the irradiated material **b** Photoluminescence mapping of irradiated part of the material (dark blue dots around the central dark blue zone)



mechanism dominates, defects are rarely created in the host material. However, at the end range of ions, where nuclear energy loss mechanism dominates, elastic collision between irradiated ions and host atoms leads to formation of defects of their complexes (Wesch and Wendler 2016; Avasthi and Mehta 2011; Sen and Akhtar 2002; Sen et al. 2000; Kumar et al. 2013). In the present work, creation of such defects leads to observed increase in the series resistance, decrease in the effective free carrier concentration and increment in the built-in potential of the selectively irradiated device.

Conclusions

In summary, Ni/4H-nSiC Schottky barrier diodes have been fabricated and irradiated selectively with 200 MeV silver ions. Compared to pristine device, the barrier height and the ideality factor in the selectively irradiated device are improved. Experimentally calculated values of interface states density revealed an order of magnitude reduction and, hence, improved interface after selective ion irradiation. Photoluminescence studies emphasized that bulk quality of the material was degraded due to the formation of defects at the end range of irradiated ions. These defects lead to decrease in effective free carrier concentration and built-in potential values in selectively irradiated device. Moreover, formed defects also cause increase in the series resistance of the irradiated device. Overall proposed technique with some modifications can be implemented in resolving the interface states issue in advanced microelectronics and other MOS devices.

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Compliance with ethical standards

Conflict of interest The authors declare no conflict of interest.

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