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Swift heavy ion irradiation induced modification of electrical characteristics of Au/n-Si Schottky barrier diode

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Abstract

Modification in the electrical transport properties of Au/n-Si(111) Schottky barrier diode (SBD) by swift heavy ion (SHI) irradiation has been investigated using in situ capacitance-voltage (C-V) and current-voltage (I-V) measurements at various irradiation fluences ranging from 1×10^{12} to 1×10^{13} ions cm⁻². The variations in various parameters of the Schottky diode have been systematically studied as a function of fluence during irradiation. The ionized-donor concentration decreases with the increase in fluence, while the ideality factor, reverse saturation current and reverse leakage current increases with fluence. The change in these parameters is explained in the light of basic energy loss mechanisms of the SHI at the metal-semiconductor (MS) interface. The Schottky barrier height (SBH) decreases from a value of $0.83 \, \text{eV}$ for the unirradiated diode to $0.66 \, \text{eV}$ for the diode irradiated with a fluence of $1 \times 10^{12} \, \text{ions cm}^{-2}$. After this fluence the SBH remains almost constant up to a fluence of $1 \times 10^{13} \, \text{ions cm}^{-2}$. The reduction in SBH is caused by an increase in interface state density at the MS interface induced by SHI irradiation. The role of electronic energy loss in modification of interface states has been envisaged in relation to the immunity of SBH over a wide fluence range after an initial fluence of $1 \times 10^{12} \, \text{ions cm}^{-2}$. © 2001 Elsevier Science Ltd. All rights reserved.

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1. Introduction

The electrical characteristics of a MS contact are extremely sensitive to interface state density at the MS interface. Ion irradiation at the interface causes modification of the interface and affects the electrical characteristics of the Schottky diode formed on the semiconductor. There have been many studies on the effect of low energy ion implantation on the electrical characteristics of Schottky barrier diodes (SBDs) [1–4]. These studies established that low energy ion implantation generally decreased the Schottky barrier heights

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(SBHs) on n-type Si and increased the barrier heights on p-type Si. But the studies on the modifications of electrical characteristics of SBDs by swift heavy ion (SHI) irradiation (having energies of a few tens to hundreds of MeV) are rather scarce in the literature [5]. An important difference in this case with respect to low energy ion implantation is the high electronic energy loss due to inelastic collisions of swift heavy ions (SHIs) at the MS interface of SBD. In case of low energy ion implantation, nuclear energy loss is the dominant energy loss mechanism whereas for SHI irradiation, electronic energy loss due to inelastic collision is two to three orders of magnitude larger than nuclear energy loss. In case of SHI the range of ion is a few tens of micro-meter (µm) and so ion goes deep into the substrate after modifying the interface unlike case of low implantation where ions get implanted close to the interface.

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The SBH of a metal on silicon is determined primarily by the MS interface states and is nearly independent of the doping concentration [6]. The SHI irradiation of the MS interface is expected to produce defect centers at the interface leading to the enhancement in density of interface states. These interface states controls the SBH and are responsible for the observed modifications in the barrier height of SBD. But here the roles of intense electronic energy loss need to be given proper consideration. The large electronic energy loss may induce effects like, mixing at the interface, modification of the microscopic inhomogeneities at the interface and annealing of the interface defects which can alter the electronic structure of the MS interface. Although the above explanation is relatively easy to comprehend, but the issue of modification of interface by SHI irradiation in silicon involves quite complex phenomena comprising of many competing processes.

To address the above-mentioned problems in a proper perspective, systematic electrical characterization of the SHI irradiated Au/n-Si(111) SBD was carried out in situ at various ion fluences on the same SBD keeping all other physical conditions like vacuum environment, temperature, etc constant. The results of the detailed investigation of current–voltage (I-V) and capacitance–voltage (C-V) characteristics of Au/n-Si(111) SBD irradiated with $100\,\mathrm{MeV}^{-16}\mathrm{O}^{7+}$ ion beam at various irradiation fluences ranging from 1×10^{12} to $1\times10^{13}\,\mathrm{ions\,cm}^{-2}$ are presented here.

2. Experimental procedure

The Schottky diode was fabricated on phosphorus-doped n-type $(0.2-0.3\,\Omega\text{-cm}$ resistivity) Si wafers of $(1\,1\,1)$ orientation. Prior to back ohmic contact and Schottky contact deposition, the Si wafer was properly cleaned and etched for native oxide removal from the surface. After this the sample was inserted in a high vacuum chamber and aluminum film of $100\,\mathrm{nm}$ thickness was deposited by resistive evaporation method on the backside of the Si wafer for ohmic contact fabrication. The base pressure of the chamber was $1\times10^{-7}\,\mathrm{mbar}$. The aluminum back ohmic contact was annealed at $525^{\circ}\mathrm{C}$ for $25\,\mathrm{min}$ in flowing argon ambient. After annealing in argon atmosphere, the sample was again loaded in the evaporation chamber to deposit a 2 mm diameter Au Schottky contact on front side of the sample.

The irradiation was performed by 100 MeV ¹⁶O⁷⁺ ion beam using the 15 UD Pelletron accelerator facility [7] at Nuclear Science Centre, New Delhi. The electrical transport studies were carried out during irradiation in a vacuum chamber at a vacuum of the order of 10⁻⁷ mbar maintained by a cryopump. The Au/n-Si

SBD was mounted on a copper sample holder and the irradiation was performed from the front Au Schottky contact side. The two electrical contacts from the diode were taken out from the irradiation chamber through shielded coaxial cables using an electrical feed-through on a flange of vacuum chamber. The I-V and C-V characteristics of the Schottky diode were carried out in situ by stopping the beam after irradiation at each fluence. The fluence was varied from 1×10^{12} to $1 \times 10^{13} \, \mathrm{ions \, cm^{-2}}$. The C-V characteristics were measured using Boonton 7200 capacitance-meter. For I-V measurements, Keithley 230 voltage source and 386 pico-ammeter were used.

3. Results and discussion

3.1. Capacitance-voltage characteristics

The C-V characteristics have been analyzed using the Schottky–Mott equation [8]

$$C = \frac{\varepsilon A}{W} = \sqrt{\frac{q\varepsilon N_{\rm D} A^2}{2(V_{\rm bi} - V - V_{\rm T})}},\tag{1}$$

where ε is the dielectric constant of the semiconductor, A is the area of the Schottky diode, W is the depletion width, $N_{\rm D}$ is the concentration of ionized donor atoms, $V_{\rm T}$ is the thermal voltage (= $k_{\rm B}T/q$), $V_{\rm bi}$ is the built-in voltage and V is the applied reverse bias. Using Eq. (1) the value of $N_{\rm D}$ may be written as

$$N_{\rm D} = \frac{2}{q\varepsilon} \left[\frac{-1}{\mathrm{d}(A^2/C^2)/\mathrm{d}V} \right]. \tag{2}$$

Hence from the slope of $1/C^2$ versus V curve the value of ionized dopant concentration $N_{\rm D}$ or free carrier concentration may be obtained. The SBH $\Phi_{\rm B}$ is related to the built-in voltage $V_{\rm bi}$ by the following equation

$$\Phi_{\rm B} = V_{\rm bi} + V_{\rm T} \ln \left(\frac{N_{\rm C}}{N_{\rm D}} \right). \tag{3}$$

Here $N_{\rm C}$ is the effective density of states in the conduction band and $N_{\rm D}$ is the donor concentration. From the intercept of the $1/C^2$ versus V curve on the voltage axis, the value of $\Phi_{\rm B}$ is calculated.

Fig. 1 shows the $1/C^2$ versus V characteristics of pristine and irradiated Au/n-Si Schottky diode. The irradiation fluence varied from 1×10^{12} to 1×10^{13} ions cm⁻² and all the C-V measurements were recorded in situ by stopping the ion beam at various fluences. The capacitance decreased as a function of fluence. For pristine SBD the value of capacitance at zero bias was 1776 pF while for the final fluence of

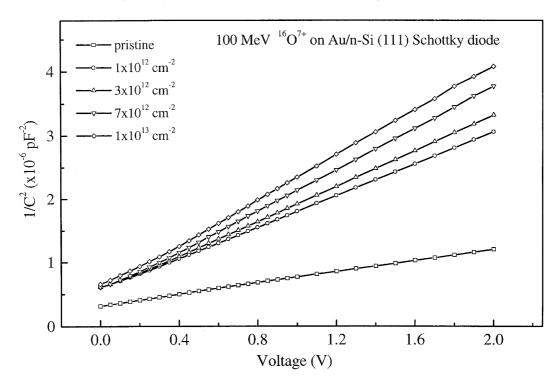


Fig. 1. The C-V characteristics of unirradiated as well as irradiated (fluence ranging from 1×10^{12} to 1×10^{13} ions cm⁻²) Au/n-Si(1 1 1) SBD.

Table 1 The ionized-donor concentration (N_D) , Schottky barrier height (Φ_B) , ideality factor (n), reverse saturation current (I_S) and reverse leakage current (I_R) of unirradiated as well as irradiated (fluence ranging from 1×10^{12} to 1×10^{13} ions cm⁻²) Au/n-Si(111) Schottky barrier diode

Fluence (ions cm ⁻²)	$N_{\rm D}$ (cm ⁻³)	$\Phi_{\rm B}(C-V)$ (eV)	N	$\Phi_{\rm B}(I-V)$ (eV)	<i>I</i> _S (μA)	I _R (at 2 V) (μA)
0	2.7×10^{16}	0.93	2.3	0.83	0.003	6.8
1×10^{12}	9.7×10^{15}	0.69	3.9	0.66	1.9	46.3
3×10^{12}	8.8×10^{15}	0.63	3.9	0.66	2.1	51.3
7×10^{12}	7.5×10^{15}	0.56	3.7	0.66	2.5	54.5
1×10^{13}	6.8×10^{15}	0.57	3.8	0.66	2.7	59.0

 $1\times10^{13} {\rm ions\,cm^{-2}}$, it decreased to 1233 pF. From the experimental $1/C^2$ versus V curves, the values of donor concentration $N_{\rm D}$ and SBH $\Phi_{\rm B}$ have been determined. The donor concentration for pristine diode was $(2.7\pm0.1)\times10^{16}\,{\rm cm^{-3}}$. It then decreased with increase in fluence and at a final fluence of $1\times10^{13}\,{\rm ions\,cm^{-2}}$, its value came down to $(6.8\pm0.3)\times10^{15}\,{\rm cm^{-3}}$. The value of SBH for the pristine diode was $0.93\pm0.03\,{\rm eV}$ and then it decreased with the rise in fluence. For a fluence of $1\times10^{13}\,{\rm ions\,cm^{-2}}$, the value of SBH de-

creased to $0.57\pm0.03\,\mathrm{eV}$. The values of donor concentration and SBH at various fluences have been given in Table 1.

In order to understand the observed modifications in the C-V characteristics, it is important to understand the implications of high energy ion irradiation at the MS interface. It is known that when a SHI penetrates a solid target, it transfers its energy to the solid through two mechanisms: (1) electronic energy loss S_e due to inelastic collision causing excitation and ionization of the atoms

of the target, and (2) nuclear energy loss S_n due to elastic collision causing displacements of the atoms from their regular lattice sites [9,10]. The elastic collision is known to create defects in the semiconductor material like vacancies, interstitials and combination/agglomeration of these defects leading to the formation of complex and stable defect structures [11–14]. From the earlier studies on SHI irradiation of Si [14], it has been reported that the most prominent defects created in the silicon are singly and doubly negative charge states of divacancy. These defects have associated deep levels present inside the band gap of Si and they act as traps for the free carriers resulting in reduction of their concentration. The deep level at $E_{\rm C} - 0.23 \, {\rm eV}$ has been identified as associated with doubly negative charge state of divacancy. The singly negative charge state of divacancy introduces a deep level situated at $E_{\rm C} - 0.43 \, {\rm eV}$ [14]. The decrease in capacitance of the Schottky diode after irradiation implies a widening in the semiconductor depletion width. Since the charge-neutrality condition at the MS interface should be satisfied, widening of the depletion width results from a reduction of the ionized-donor concentration after SHI irradiation. This is confirmed from the C-V measurements. In fact the ionized donor concentration decreases from

 $(2.7\pm0.1)\times10^{16}\,\mathrm{cm}^{-3}$ for the pristine diode to $(6.8\pm0.3)\times10^{15}\,\mathrm{cm}^{-3}$ for same diode when irradiated at a fluence of $1\times10^{13}\,\mathrm{ions\,cm}^{-2}$. A schematic diagram depicting a possible model to explain the observed behavior is shown in Fig. 2. One of the mechanisms causing a decrease in the net ionized donor concentration is the existence of negatively charged deep defect centers as has been shown by many authors using DLTS measurements. Due to the presence of these centers, some of the positive shallow donors in the depletion region are compensated so that the effective net ionizeddonor concentration is decreased. The donor compensation causes widening of the depletion width so that the charge-neutrality condition is maintained at the MS interface. The increase in the depletion width results in decrease in the Schottky diode capacitance as can be seen from Eq. (1).

3.2. Current-voltage characteristics

The I-V characteristics have been analyzed using the thermionic emission equation [15], which is given by

$$I = I_{\rm S} \left[\exp\left(\frac{qV}{nk_{\rm B}T}\right) - 1 \right],\tag{4}$$

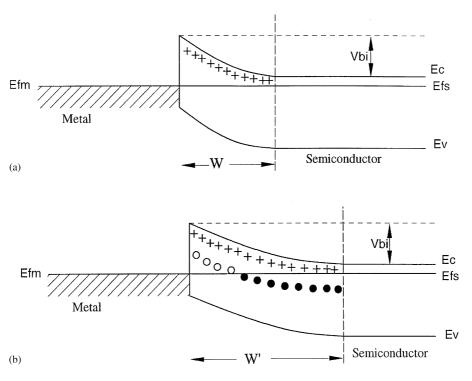


Fig. 2. The effect of donor-charge compensation by negative charge centers on the depletion width has been shown schematically. (a) The band diagram of SBD when charged defects are not present at the interface. (b) The increase in the depletion width due to donor charge compensation.

where

$$I_{\rm S} = AA^{**}T^2 \exp\left(\frac{-q\Phi_{\rm B}}{k_{\rm B}T}\right),\tag{5}$$

$$\Phi_{\rm B} = \frac{k_{\rm B}T}{q} \ln\left(\frac{AA^{**}T^2}{I_{\rm S}}\right). \tag{6}$$

Here I_S is the reverse saturation current, A the area of the Schottky diode, A^{**} the effective Richardson constant (taken as $10 \,\mathrm{A\,cm^{-2}\,K^{-2}}$), T is the absolute temperature, n the ideality factor, k_B the Boltzmann's constant, q the electronic charge, Φ_B the SBH. From the slope of $\log I$ versus V curve, the value of ideality factor is calculated. The I_S is determined from the intercept of $\log I$ versus V curve on the y-axis. Putting this value of I_S in Eq. (6), the value of SBH is evaluated.

Fig. 3 shows the I-V characteristics for pristine as well as irradiated Schottky diode at various fluences ranging from 1×10^{12} to $1\times10^{13}\,\mathrm{ions\,cm^{-2}}$. The I-V characterization was performed in situ by stopping the beam at various fluences and keeping all other parameters, e.g. ion flux, vacuum environment and sample temperature, identical. For pristine Schottky diode the ideality factor n was found to be 2.3 ± 0.1 . After irradiation with a fluence of $1\times10^{12}\,\mathrm{ions\,cm^{-2}}$, the

value of ideality factor increased to 3.9 ± 0.1 . Then it remained almost constant at this value up to a fluence of 1×10^{13} ions cm⁻². The reverse saturation current $I_{\rm S}$ for the pristine SBD was $3 \times 10^{-3} \,\mu\text{A}$. It then increased with the fluence and for a final fluence of $1 \times 10^{13} \, \mathrm{ions} \, \mathrm{cm}^{-2}$ its value was 2.7 µA. Similarly, the reverse leakage current I_R (at 2 V) also increased from a value of 6.8 μ A for the pristine SBD to a value of 59.0 µA for the final fluence of 1×10^{13} ions cm⁻². The reverse I-V characteristics for the Schottky diode for unirradiated as well as irradiated SBD are shown in Fig. 4. It is clear from Fig. 4 that as the fluence increases the reverse characteristics of the Schottky diode deteriorates with regard to its rectifying behavior. The increase in reverse leakage current is due to irradiation induced defects of the MS interface that enhances the defect assisted tunneling. The variations of ideality factor, reverse saturation current and reverse leakage current with the fluence are summarized in Table 1.

The behavior of SBH with fluence of $100 \, \text{MeV}^{16} \text{O}^{7+}$ ion beam may be explained as follows. When the SHI penetrates through the MS interface, it loses the energy through nuclear and electronic energy loss mechanisms. The variation of nuclear (S_n) and electronic (S_e) energy losses as a function of depth inside the Au/n-Si Schottky diode is shown in Fig. 5. It is clear from the figure that

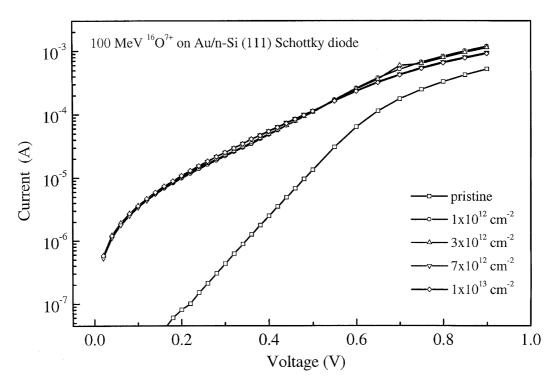


Fig. 3. Forward I-V characteristics of unirradiated as well as irradiated (fluence ranging from 1×10^{12} to 1×10^{13} ions cm⁻²) Au/n-Si(1 1 1) SBD.

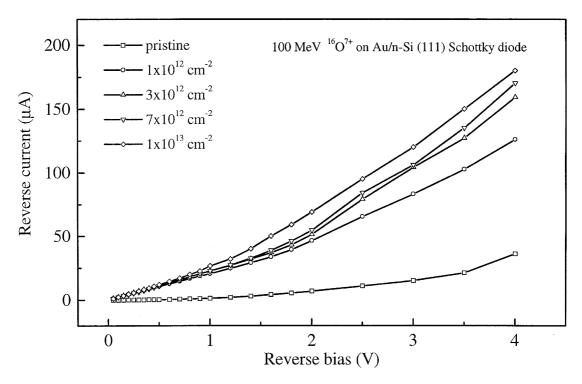


Fig. 4. Reverse I-V characteristics of unirradiated as well as irradiated Au/n-Si(111) SBD.

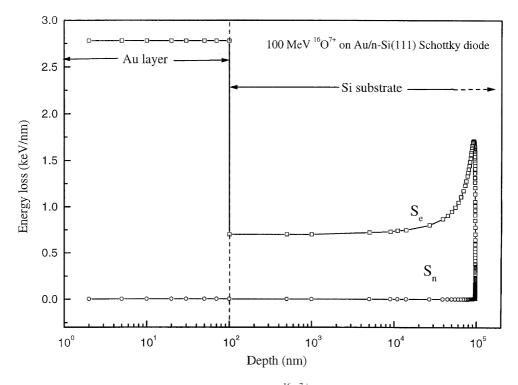


Fig. 5. Variation of electronic and nuclear energy losses of 100 MeV ¹⁶O⁷⁺ ion with depth inside Au/n-Si(111) Schottky diode.

near the MS interface Se is the dominant energy loss mechanism being about 1600 times larger than S_n . At the MS interface, the average values of electronic (S_e) and nuclear (S_n) energy losses are 1.74 and 0.11 \times $10^{-2} \,\mathrm{keV/nm}$, respectively. In top 100 nm Au layer, the values of S_e and S_n are 2.78 and $0.17 \times 10^{-2} \,\text{keV/nm}$ while in silicon near the MS interface the values of S_e and S_n are 0.69 and $0.04 \times 10^{-2} \text{ keV/nm}$, respectively. All these energy loss calculations have been performed using SRIM-98 [10] simulation program. The intense electronic excitation due to predominant inelastic collision of the SHI at the MS interface region leads to the production of vacancies, interstitials and complex defects. The SHI irradiation results in the introduction of interface states at MS interface which influence the SBH [16,17]. Due to strong screening by the charge carriers in metals, top Au-layer of SBD is not affected by electronic excitation. According to the Fermi level pinning model of Bardeen [18], when the interface density D_S is very high, the SBH of SBD on an n-type semiconductor in the so-called Bardeen limit is given by

$$\Phi_{\rm BB} = (E_{\rm g}/q - \Phi_0) - \Delta\Phi,\tag{7}$$

where $E_{\rm g}$ is the band gap of the semiconductor, $q\Phi_0$ is the energy level in coincidence with the Fermi level before the MS contact was formed (also called the neutrality level), and $q\Delta\Phi$ is the lowering of the Schottky barrier due to image force (it being of the order of 0.01 eV may be neglected). On the other hand, when $D_{\rm S}$ is zero, then the SBH of SBD on an n-type semiconductor in the so-called Schottky limit [19] is given by

$$\Phi_{\rm BS} = \Phi_{\rm m} - \chi - \Delta \Phi, \tag{8}$$

where $\Phi_{\rm m}$ is the work function of the metal and χ is the electron affinity of the semiconductor. According to Sze [15], $q\Phi_0 = 0.30 \pm 0.36 \,\text{eV}$, $q\chi = 4.05 \,\text{eV}$, $E_g =$ 1.12 eV for Si at $T = 300 \,\mathrm{K}$, and $q\Phi_{\mathrm{m}} = 5.1 \,\mathrm{eV}$ for Au. Using these values the estimated values of $q\Phi_{\rm BB}$ and $q\Phi_{\rm BS}$ are 0.82 ± 0.36 and $1.05\,{\rm eV}$, respectively. This means that when the interface state density D_S increases from the Schottky limit to the Bardeen limit, the SBH should decrease from 1.05 to $0.82\pm0.36\,\mathrm{eV}$. From the I-V characteristics for pristine diode we have calculated the SBH as 0.83 ± 0.01 eV. This means that there is a finite density of interface states D_S existing at the Au/n-Si(111) interface for the unirradiated sample. The SBH decreased to a value of $0.66 \pm 0.01 \, eV$ at an irradiation fluence of $1 \times 10^{12} ions cm^{-2}$. After this fluence it remained constant at $0.66 \pm 0.01 \, \text{eV}$ upto a fluence of $1 \times 10^{13} \, \text{ions cm}^{-2}$ as shown in Table 1. The observed decrease in SBH of Au/n-Si Schottky diode after SHI irradiation correlates well with the increase in interface state density and the resultant orientation of the Schottky barrier more towards the Bardeen limit. As the SHI passes through the SBD it produces strong

ionization of the target atoms near the MS interface due to large electronic energy loss ($S_e = 1.74 \,\text{keV/nm}$, $S_{\rm e}/S_{\rm n} \approx 1600$) at the MS interface. During their relaxation, the electronic excitations can produce several specific structure defects and phase transitions [20,21] as well. Since the electronic energy loss entirely determines the energy dissipation of fast ions, so it is natural to expect a noticeable influence of lattice ionization in the evolution of the irradiated area including mechanisms of defect production and impurity distribution [22,23]. In fact in a single crystalline Si the effect of very efficient annealing of the defects previously introduced by protons is observed as a result of 340 MeV Xe ion irradiation for the fluence of 10¹² ions cm⁻² [24]. In a recent study [25], Motooka et al. observed annealing of the point defects due to electronic energy loss when a single crystalline silicon wafer was irradiated with 5 MeV Si ion beam. In the present investigation it is seen that after a fluence of $1 \times 10^{12} \, \text{ions cm}^{-2}$ the rate of creation of defects gets balanced by the rate of annealing of defects at the MS interface by electronic excitation/ionization of the target atoms [26,27] up to a fluence of 1×10^{13} ions cm⁻². The irradiation initially causes an increase in the interface state density leading to decrease in the SBH at an irradiation fluence of $1 \times 10^{12} \, \text{ions cm}^{-2}$. After this fluence the effect of annealing of the defects causes the interface state density to remain rather constant and hence the SBH also remains unaltered up to a fluence of $1 \times 10^{13} \, \text{ions cm}^{-2}$ which is an order of magnitude higher.

4. Conclusion

The Au/n-Si(111) SBD was irradiated by 100 MeV $^{16}\text{O}^{7+}$ ion beam. In situ C-V and I-V measurements were performed to investigate the modifications of electrical characteristics of Schottky diode by SHI irradiation. Systematic modification in various parameters of the Schottky diode like ideality factor, reverse saturation current and reverse leakage current is indicative of the introduction of SHI irradiation induced defects at the MS interface. The SBH for the unirradiated Schottky diode decreased from 0.83 to 0.66 eV after irradiation at a fluence of 1×10^{12} ions cm⁻². After this fluence it did not vary considerably over a large range up to a fluence of 1×10^{13} ions cm⁻². The increase in interface state density caused the Schottky barrier to move from Schottky limit to Bardeen limit resulting in initial reduction in SBH. The dynamic balancing of defect creation and annihilation process by intense electronic excitation at the MS interface after a fluence of 1×10^{12} ions cm⁻² leads to the immunity of the SBH over a larger range of irradiation up to a fluence of $1 \times 10^{13} \, \text{ions cm}^{-2}$.

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