4.1 INTRODUCTION

The heavy ion irradiation is a preferred method in controlled reduction of the minority carrier’s lifetime in silicon power devices, formation of deep buried layers, and introduction of controlled amount of defects in semiconductors [1-3]. These increasing interests of ion beams in processing technologies motivate the importance in studies of defects induced by irradiations of heavy ions in semiconductors. It is well known that low energy ion implantation leads to degradation of Schottky diode parameters with increasing fluence [4-6]. It is found by our research group at MeV energies swift heavy ion irradiation of silicon diodes results in saturated values of barrier height and other parameters after a critical ion fluence [7, 8] as discussed in Chapter 3. As described earlier in Chapter 1, the important difference of swift heavy ion irradiation with respect to low energy ion implantation is the high electronic energy loss due to inelastic collisions of swift heavy ions in materials, which are initially two to three orders of magnitude larger than nuclear energy loss due to elastic collisions. This high electronic energy loss produces a strong ionization of target atoms all
along the trajectory. In case of swift heavy ions, the range of ions are a few tens of micrometer and so ion goes deep into the substrate after modifying the interface unlike the case of low energy implantation where ions get implanted close to the interface. It is well established that ion irradiation into semiconductors causes structural damage, which in turn results in electrically active defects. These electrically active defects produced in Si can result in pinning of Fermi level to a dominant deep level [9, 10]. The Fermi level pinning may be within a region of a few nanometers around a heavy ion track and can result in formation of a nanosized channel with a modified Fermi level embedded in bulk silicon [10]. Such nanochannels can act as electronic nanowires due to local Fermi level modification that induces a bending of the electronic bands around the ion track. The technological advantage of such nanochannels is that, unlike the traditional nanowires, these ion induced nanochannels are readily embedded into the Si crystal. Besides these important applications, ion irradiation studies are interesting from the viewpoint of fundamental understanding of a whole range of solid state phenomena. There have been a lot of studies on defects produced by low energy ion implantation in silicon [11-18], but defects induced by swift heavy ions are not studied extensively. The aim of present work is to study systematically the role of this high electronic energy loss in evolution of defects and correlate them with the electrical characteristics of the materials. In particular, in situ deep level transient spectroscopy (DLTS) allowed us to monitor the evolution of irradiation induced defects as a function of irradiation fluence. Generally, there are variations in electrical characteristics from sample to sample even the diodes fabricated on the same wafer. So, to study precisely effect of ion irradiation as a function of ion fluence, the DLTS experiment has been carried out in situ on the same sample.

In this Chapter, studies on in situ DLTS and current-voltage (I-V) characterization of swift heavy ion irradiated Au/n-Si (100) Schottky barrier diode carried out on the single
diode keeping all other physical conditions like ion flux, temperature and vacuum environment identical are presented. The results of the detailed investigation of in situ electrical characterization at various irradiation fluences ranging from $5 \times 10^9$ to $1 \times 10^{12}$ ions-cm$^{-2}$ are presented in section 4.3 and discussed section 4.4.

4.2 EXPERIMENTAL DETAILS

The sample used in present study was Au/n-Si (100) Schottky barrier diode. The Schottky diodes were fabricated by using of n-type Si (100) both side mirror polished sample of resistivity 1-10Ω-cm. The Schottky contacts were created by deposition of Au on the sample having Ohmic contact by electron beam heating technique in an ultra high vacuum chamber. The complete process is described in detail section 2.3 of Chapter 2. A 100 nm Au layer was deposited through a stainless steel mask having contact diameter of 2 mm at a base pressure of $10^{-8}$ mbar region. The ion irradiation was performed at room temperature by 100 MeV $^{28}$Si$^{7+}$ ion beam using the 15UD Pelletron accelerator [19] facility at Inter-University Accelerator Centre, New Delhi. Si ion beam was chosen to avoid the introduction of impurity atom deep into Si substrate. The irradiation fluence was varied from $5 \times 10^9$ to $1 \times 10^{12}$ ions cm$^{-2}$. During irradiation the beam current was 4.0 nA corresponding to ion flux of $3.1 \times 10^9$ ions-cm$^{-2}$sec$^{-1}$ to avoid sample heating. A Boonton 7200 capacitance meter based computer controlled DLTS system was used for the present study. Five DLTS spectra with rate windows between (115 s)$^{-1}$ and (2310 s)$^{-1}$ were simultaneously recorded during one single temperature scan from 80K to 300K after each irradiation fluence by stopping the ion beam in beam line. The current-voltage ($I-V$) measurements were carried out with a programmable Keithley 2400 source meter. All measurements were carried out at various stages of irradiation in the experimental chamber maintained at a vacuum of $\sim 10^{-7}$ mbar.
4.3 RESULTS

4.3.1 Current-voltage measurements

The in situ $I$-$V$ characteristics for the unirradiated and irradiated Au/n-Si Schottky diode up to an ion fluence value of $1 \times 10^{12}$ ions cm$^{-2}$ are shown in Figure 4.1. In case of a moderately doped semiconductor, thermionic emission is the dominant current transport mechanism across the barrier at room temperature. From a fit of linear region of the forward bias semilogarithmic $I$-$V$ curve to Eq.(3.1) of Chapter 3, the values of Schottky barrier parameters were determined.

For the unirradiated diode the barrier height was 0.80eV. The ideality factor for as-prepared diode was 1.1. After irradiation at a fluence of $5 \times 10^9$ ions-cm$^{-2}$, the barrier height decreases to a value of 0.72eV without any significant change in ideality factor. Thereafter, the barrier height decreases further reaching a value of 0.67 eV with ideality factor 1.23 for irradiation fluence $1 \times 10^{11}$ ions-cm$^{-2}$. Beyond this ion fluence, Schottky barrier height remains immune to further irradiation up to the highest irradiation fluence used. The variation of barrier height as a function of irradiation fluence is shown in Figure 4.2. This behavior is quite in good agreement with the results found in previous Chapter 3 for Au/n-Si(100) Schottky diodes [7, 8]. The ideality factor increases from a value of 1.10 to 1.25 after ion irradiation at fluence $1 \times 10^{12}$ ions-cm$^{-2}$.

The leakage current (measured at -2V) remained almost unchanged after low fluence ion irradiation with respect to the as-prepared sample, and increased at higher fluences. The leakage current increases from a value of $9.8 \times 10^{-7}$A for unirradiated diode to $4.9 \times 10^{-6}$A after irradiation at fluence of $1 \times 10^{12}$ ions-cm$^{-2}$. The increase in value of leakage current is associated with irradiation induced defects. In Chapter 3, the decrease of barrier height,
Figure 4.1: Experimental current-voltage characteristics of the Au/n-Si (100) Schottky diode at different irradiation fluences.

Figure 4.2: Irradiation fluence dependence of the Schottky barrier height for Au/n-Si Schottky structure.
increase of ideality factor and leakage current were explained in terms of an increase in interface state density due to defects at the interface [7, 8]. In previous Chapter 3, it has been shown that density of interface states due to defects increases at lower fluences and saturate at higher fluences [7].

4.3.2 Deep level transient spectroscopy measurements

In order to develop deeper understanding of the influence of defects on the electrical characteristics, the creation and evolution of irradiation-induced defects in the Au/n-Si(100) structure were monitored by means of DLTS technique. DLTS is a high frequency capacitance transient method useful for observing a wide variety of deep defects in semiconductor devices [21]. DLTS spectrum is a plot of difference in capacitance ($\delta C$) versus temperature. The trap concentration ($N_T$) can be determined by knowing peak height ($\delta C_{max}$) in the DLTS spectrum. The time constant ($\tau$) for the capacitance transient, activation energy ($E_C - E_T$) and capture cross-section ($\sigma$) of the deep level are related as [22]

$$\tau \tau^2 = \frac{\exp\left(\frac{(E_C - E_T)}{kT}\right)}{\gamma \sigma},$$

(4.1)

where $\gamma$ is the material coefficient and is defined as

$$\gamma = \frac{16\pi m^*_e k^2}{gh^3},$$

(4.2)

where $m^*_e$ is the electron effective mass, $h$ is Plank’s constant and $g$ is degeneracy factor. The $\gamma$ value for n-Si is $1.07 \times 10^{21}$ cm$^{-2}$s$^{-1}$K$^{-2}$. The slope of the Arrhenius plot $\ln(\tau T^2)$ versus $(1000/T)$ yields the activation energy of the defects and intercept on y axis $\ln[(1/\sigma\gamma)]$ gives the capture cross section ($\sigma$).
Figure 4.3 shows the DLTS spectrum for unirradiated Au/n-Si (100) Schottky structure at different rate windows. Arrhenius plot for the unirradiated diode is shown in Figure 4.4. Two dominant DLTS peaks $E_1(E_c-0.23\,eV)$, and $E_2(E_c-0.40\,eV)$ are present in unirradiated samples. These are identified as the doubly negative divacancy, $V_2(=\cdot\cdot\cdot)$ and the singly negative divacancy, $V_2(-/\cdot\cdot\cdot)$, respectively [23-26]. Near interface damage introduced during the fabrication of Schottky barrier diodes by electron beam deposition of metals on $n$-type silicon produces these defects [23].

Figure 4.5 shows the DLTS spectra for ion irradiated Au/n-Si (100) SBD in the fluence range $5\times10^9$ to $1\times10^{12}$ ions cm$^{-2}$. The level $E_1$ at $E_c-0.23\,eV$ due to $V_2(=\cdot\cdot\cdot)$ remain nearly same after irradiation while an increase in the height of peak of $E_2$ is observed up to an irradiation fluence of $5\times10^{10}$ ions-cm$^{-2}$. After a fluence value of $5\times10^{10}$ ions-cm$^{-2}$ peak height starts decreasing for the further irradiation fluences. It is observed that a new level $E_3$ at $E_c-0.32\,eV$ is generated during swift heavy ion irradiation after a fluence of $5\times10^9$ ions cm$^{-2}$. There is a slight shift in the position of peaks towards higher temperature with increasing irradiation fluence. Interestingly, it is found that the height of DLTS peak of $E_3$ level remains same with increasing irradiation fluence. The variation of trap concentration of divacancies $V_2(-/\cdot\cdot\cdot)$ with ion irradiation fluence is shown in Figure 4.6. One can see that initially trap concentration increases but after a fluence of $5\times10^{10}$ ions-cm$^{-2}$ trap concentration decreases with increasing ion irradiation fluence.

4.4 DISCUSSION

The implication of high-energy ion transport through the Au/n-Si Schottky diode is necessary to understand to realize the observed behavior. As discussed in detail in Chapter 1,
Figure 4.3: DLTS spectra of unirradiated Au/n-Si (100) Schottky diode at different rate windows.

Figure 4.4: Arrhenius plot for unirradiated Au/n-Si (100) Schottky diode.
Figure 4.5: DLTS spectra of unirradiated and irradiated Au/n-Si (100) Schottky diode at different ion irradiation fluences (y-scale is inverted).
when 100 MeV $^{28}$Si$^{7+}$ ion passes through the metal-semiconductor interface, it losses energy by two nearly independent processes: (1) elastic collisions of the ion with the target atoms known as nuclear energy loss ($S_n$), and (2) inelastic collisions of the highly charged projectile ion with the atomic electrons of the materials known as electronic energy loss ($S_e$). In this case, electronic energy loss is the dominant energy loss process at the interface and $S_n$ dominants only at the end of ion range as shown in Figure 4.7. All energy loss calculations have been performed using standard Monte Carlo simulation program [27] called SRIM-2006. It is well established that $S_n$ causes creation of defects like vacancies, interstitials and combination/agglomeration of these defects leading to form complex and stable defect structures [28] while $S_e$ produces strong ionization of the target atoms along its trajectory. During their relaxation, the electronic excitation can produce several specific structural defects and phase transitions [29, 30]. The Au layer is not affected due to the strong screening of charges in metals.

Two theoretical models thermal spike [31] and coulomb explosion [32], are used to explain the local excitation of the lattice by energy transfer from the highly excited electronic system to the lattice atoms as described in Chapter 1. Both mechanisms can result in materials modification depending on the properties of the materials and deposited energy density [33, 34]. According to the widely used thermal spike model [31] rapid energy transfer through electron phonon coupling makes the system abnormally excited and the region around the ion track gets suddenly heated to a very high temperature within a small time scale [35]. The temperature evolution of the ion track for 100 MeV Si$^{7+}$ ions in silicon is above 800K [36].
Figure 4.6: Trap concentration for $V_{ZF}$ level as a function of 100 MeV $Si^{7+}$ ion irradiation fluence.

Figure 4.7: The nuclear and electronic energy losses of 100 MeV $^{28}Si^{7+}$ ions as function of depth inside Au/n-Si (100) Schottky diode.
In present case 100 MeV Si$^{7+}$ ions irradiation produces a deep level at $E_3$ ($E_C-0.32$eV). This level has been reported previously, after proton irradiation and is identified as hydrogen related defect [11, 12, 15]. The ion irradiation produced defects are enhanced by hydrogen resulting in the formation of weak Si-H bonds at the defect sites, which is dissociated at around 150°C. The released hydrogen atoms interact with the irradiation induced defects to form electrically active centers [37]. In this case hydrogen was not deliberately introduced or implanted but experimentally it is found that the hydrogen content in crystalline silicon by far exceeds the estimated equilibrium concentration [12]. It had been shown that during the annealing of Si ions implanted silicon, the formation of $E_C-0.32$ eV level is associated with the annealing of $E_C-0.23$eV level [12]. In this case region around the ion trajectory goes to very high temperature than that required to release the hydrogen atoms. These hydrogen atoms interact with irradiation-induced defects to form electrically active centers. The level at $E_C-0.32$eV gets saturated with increasing ion fluence due to the fact that the concentration of hydrogen in silicon is limited, which results in saturation at higher irradiation fluences. This released hydrogen can also interacts with divacancies V(-/0) to passivate the defects, which becomes electrically neutral and modify the Schottky barrier height [38]. It is also established that despite the impurities like oxygen and carbon atoms being potential annihilation centers. The localized disordered zones created by ion irradiation act as sinks and annihilate diffusing point defects like the divacancy centers [10]. Since the divacancies anneal out at higher fluences, so $E_3$ mainly influence the electrical characteristics, and can results in a saturated value of interface states density at the interface.

According to Bardeen’s Fermi level pinning model [39], if the interface density $D_S$ is very high, the Schottky barrier height on an $n$-type semiconductor is given by

$$\Phi_{bb} = \left(\frac{E_C}{q} - \Phi_0\right) - \Delta \Phi$$  \hspace{1cm} \text{(Bardeen limit)} \hspace{1cm} (4)
where $E_g$ is the band gap of the semiconductor, $q\Phi_0$ is the energy level coincidence with the Fermi level before the metal-semiconductor contact was formed and $q\Delta \Phi$ is the lowering of the Schottky barrier due to the image force. On the other hand, when $D_S$ is zero, then the barrier height of a Schottky barrier diode on an $n$-type semiconductor is given by

$$\Phi_{BS} = \Phi_M - \chi - \Delta \Phi$$  \hspace{1cm} \text{(Schottky limit)} \hspace{1cm} (5)$$

where $\Phi_M$ is the work function of the metal and $q\chi$ is the electron affinity of the semiconductor. According to Sze [40] $q\Phi_0 = 0.30 \pm 0.36$ eV, and $q\chi = 4.05$ eV, $E_g = 1.12$ eV for Si at 300 K, and $q\Phi_M = 5.1$ eV for Au. Using these values, the estimated values of $q\Phi_{BB}$ and $q\Phi_{BS}$ are $0.82 \pm 0.36$ eV and $1.05 \pm 0.36$ eV, respectively. This means that when interface state density $D_S$ increases from the Schottky limit to the Bardeen limit, the barrier height should decrease. From the forward bias $I$-$V$ characteristics for unirradiated diode, the calculated barrier height is $0.80 \pm 0.01$ eV. This implies that there is a finite density of interface states $D_S$ existing at the Au/$n$-Si(100) interface for unirradiated sample. This is confirmed by DLTS measurements that there are finite concentrations of divacancies in unirradiated samples, which cause of interface states. High energy ion irradiation releases the hydrogen in silicon, which produces deep level defect complexes ($E_C - 0.32$) and passivate the localized defects at the interface like divacancies $V(\sim 0)$. The barrier height decreases after irradiation, which correlate well with an increase in interface states density due to deep level defects. These defects cause an increase in the defect assisted tunneling of free electron, which results in an increase in reverse leakage current. After a particular fluence the concentration of divacancies become very less compared to $E_3$, and $E_3$ become saturate due to limited supply of hydrogen in silicon. The saturation in defect concentration results in a saturated value of interface states density, which leads to a saturated value of barrier height with respect to ion fluence.
4.5 CONCLUSIONS

In this Chapter, the defects induced by 100 MeV Si$^{7+}$ irradiation and their influence on electrical characteristics in Au/n-Si (100) Schottky structure by using combined in situ DLTS and $I$-$V$ measurements have been studied. Unirradiated structure have two dominant deep defect levels at $E_c-0.23$, and $E_c-0.40$ eV respectively due to $V_2 (=/-)$ and $V_2 (-/0)$. We have demonstrated that hydrogen related defect complex $E_3 (E_C-0.32eV)$ is formed after swift heavy ion irradiation. Due to limited concentration of hydrogen in silicon, the concentration of $E_3$ saturate at higher irradiation fluence. This defect complex has strong influence on electrical characteristics of Au/n-Si Schottky diode and causes saturation in barrier parameters at higher fluences.
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