3.1 INTRODUCTION

Metal-semiconductor (MS) structure is one of the important research tools in the characterization of semiconductor materials. Fabrication of these structures plays a crucial role in construction of some useful devices [1]. In present research program our prime interest is to study the formation and modification of potential barrier at metal-semiconductor interface. The position of the Fermi level within the semiconductor band gap determines the height of this potential barrier. In general the exact position of the Fermi level depends on the properties of the interface. At an ideal, defect free interface, the barrier height is determined by the charge neutrality level of the metal induced gap states (MIGS) [2, 3]. These states (MIGS) originate from the tails of the metal wave functions into the semiconductor. These states are predominantly donor-like close to the valance band maximum while they are predominantly acceptor-like close to the conduction band minimum. The crossover between both types is known as the charge neutrality level. Alignment of this level with the Fermi
level of the metal is required for the charge neutrality and therefore it determines the barrier height. Any chemical reaction or imperfections at the interface is not considered in this model. In addition to the MIGS, defects can exist at the MS interface and generates interface states. The electrical characteristics of Schottky contacts are very sensitive to the defects at the MS interface. Energetic ion irradiation is one of the mechanisms able to modify the barrier characteristics of MS interface. When an energetic ion passes through the semiconductor it produces various types of defects [4]. These defects give rise to additional discrete levels in the band gap (possibly deep levels) and the Fermi level can pinned to one of these levels, possibly quite far from the charge neutrality level. There are some reports in literature [5-7] on the effect of ion implantation on the electrical characteristics of Au/n-Si (100) Schottky barrier diode but modifications of Au/n-Si (100) Schottky barriers induced by high energy swift heavy ions (heavy ions having velocity comparable to Bohr velocity of electron in the orbit) irradiation have not been studied extensively. In swift heavy ions the electronic energy loss $S_e$ due to inelastic collisions is two to three orders of magnitude larger compared to nuclear energy loss $S_n$ due to elastic collisions. This large electronic energy loss may lead to phenomena like, mixing at interface, modification or introduction of the microscopic inhomoginities at the interface and annealing of the interface defects that can alter the electronic structure of the MS interface. The studies on the effect of swift heavy ion irradiation on Schottky barrier diodes are important for fundamental understanding of the phenomenon of ion-solid interaction at the interface as well as its application. In some fields such as the testing of radiation hardness for aerospace industry [8] and the development of particle detectors [9], it is extremely important to correlate the effects of ion irradiation on the material properties with the modification of the electrical characteristics of Schottky barriers. Moreover, swift heavy ion irradiation is useful in some applications like controlled reduction
of the minority carrier lifetime in silicon power devices, formation of deep buried layers, and introduction of controlled amount of defects in semiconductors [10-12]. These studies shed light on the basic ion-solid interaction processes, and their influence on various properties of semiconductors. The modifications induced by swift heavy ion irradiation at the MS interface can be investigated by studying electrical behavior of a Schottky diode.

Since varying the temperature is the easiest way of varying the band gap in the semiconductor, the investigation of temperature dependence of Schottky barrier height (SBH) is very helpful to understand the problem of Fermi level pinning in a certain MS contact. When the Fermi level is pinned to the charge neutrality level, the temperature dependence of the barrier height is controlled by the temperature dependence of the band gap, the direct gap as well as indirect gap [13, 14]. However if the Fermi level is pinned by defects their ionization entropy would govern the temperature dependence of the barrier height [15]. Since the temperature dependence of the band gap is much larger than that of the ionization entropy, measurements evolution allow one to distinguish between both pinning mechanisms. Although some authors [16-18] considered the origin of the Fermi level pinning such as contamination in the interface and deep impurity level but to the best of our knowledge such type of defects never identified in silicon. The temperature dependence of the Schottky barrier height in the Au/n-Si contacts is almost identical to that of the band gap in silicon [19].

In this chapter, we present the results of the detailed investigation of I-V characteristics of Au/n-Si Schottky diode irradiated with 180 MeV $^{107}$Ag$^{14+}$ ion beam at various irradiation fluences ranging from $5 \times 10^9$ to $5 \times 10^{12}$ ions-cm$^{-2}$. The ion fluences were chosen in order to rule out the possibility of ion beam mixing at the interface. Irradiation with higher fluences may result in ion beam mixing at interface or phase formation [20], which
drastically affects the barrier properties. In Section 3.3.1, a systematic *in situ* I-V characterization of the swift heavy ion irradiated Au/n-Si Schottky diode and changes in electrical characteristics after each ion fluence is discussed. Section 3.3.2 deals with the temperature dependent barrier characteristics of swift heavy ion irradiated Au/n-Si Schottky diode.

### 3.2 EXPERIMENTAL DETAILS

The substrate used to fabricate the Schottky diodes in this experiment was mirror-polished n-type Si (100) of resistivity 0.5-1.0 Ω-cm (doping concentration $1 \times 10^{15}$ cm$^{-3}$) that have an area of 5mm×5mm and thickness 275 Ωm. The Au Schottky contact was deposited on the wafer having Al Ohmic contact. The diameter of Schottky contact was 2 mm and thickness was 100nm. The details of the complete Schottky diode fabrication process has been given in section 2.3 of Chapter 2. The ion irradiation was performed at room temperature by 180 MeV $^{107}$Ag$^{14+}$ ion beam using the 15UD Pelletron accelerator facility at Inter-University Accelerator Centre, New Delhi [21]. The irradiation fluence was varied from $5 \times 10^9$ to $5 \times 10^{12}$ ions cm$^{-2}$. The irradiation was carried out *in situ* in wide fluence range on the same Schottky diode keeping all other physical conditions like sample, ion flux, temperature and vacuum environment identical. To study the true effect of ion irradiation it is necessary that the fluence dependence study should be done on the same sample because the effect of irradiation depends on the initial conditions of the samples. During irradiation the beam current was 4.0 nA corresponding to $3.1 \times 10^9$ ions-cm$^{-2}$sec$^{-1}$ to avoid the excessive sample heating. The current-voltage (I-V) measurements were carried out with a programmable Keithley 2400 source meter. The capacitance-voltage (C-V) measurements were carried out at
1 MHz by using Boonton 7200 capacitance meter. All of the measurements were carried out in a vacuum of 10^{-7} mbar.

The temperature dependent \textit{I-V} and \textit{C-V} measurements of irradiated diodes were carried out at varying temperature from 300K to 50K. Cooling was performed with a close cycle He refrigerator. The temperature was controlled by a stabilization loop consisting of a temperature diode, a heating resistance and a Lakeshore temperature controller, which regulates the temperature to a preset value. The variation of temperature was better than ±0.5 K during each temperature point of measurement. Offline temperature dependent measurements were carried out in a vacuum of 10^{-3} mbar region.

3.3 EXPERIMENTAL RESULTS AND DISCUSSION

3.3.1 Swift heavy ion irradiation of Au/n-Si (100) Schottky barrier structure

3.3.1.1 Current-voltage measurements

The \textit{in-situ} \textit{I-V} characteristics of unirradiated and irradiated Au/n-Si (100) Schottky contact in the fluence range 5\times10^9 to 5\times10^{12} ions cm^{-2} are shown in Figure 3.1. The \textit{I-V} curves at various fluences have been analyzed within the framework of thermionic emission theory as discussed in subsection 2.2.1 of Chapter 2. The experimental data is fitted with the thermionic emission equation, which is given by [22]

\[ I = I_0 \left[ \exp \left( \frac{q(V - IR_s)}{nkT} \right) - 1 \right] \]  \hspace{1cm} (3.1)

where \( I_0 \) is the saturation current and \( n \) is the ideality factor. The ideality factor \( n \) is introduced to take into account the deviation of the experimental \textit{I-V} data from the ideal
Figure 3.1: Experimental current-voltage characteristics of the Au/n-Si(100) Schottky diode at different irradiation fluences.

thermionic model. Its value should be one for an ideal contact. This deviation arises from the presence of surface charges and image force effects. The saturation current $I_0$ is given by

$$I_0 = AA'T^2 \exp \left( -\frac{q\Phi_{B0}}{kT} \right)$$

(3.2)

where $A'$, $A$, and $\Phi_{B0}$ represent the Richardson constant, the contact area ($3.14 \times 10^{-2}$ cm$^2$) and zero-bias Schottky barrier height, respectively. Other symbols in the above equations have their usual meaning.
The value of Schottky barrier height is evaluated at each temperature putting this value of \( I_0 \) in equation

\[
\Phi_{B0} = \frac{kT}{q} \ln\left( \frac{A^*T^2}{I_0} \right).
\]

(3.3)

Schottky barrier height for as prepared sample is 0.74±0.01 eV. This low value of barrier height may be due to the presence of a non-uniform thin oxide layer at the interface (related to device fabrication process) [23, 24]. The barrier height decreases with increasing irradiation fluence and becomes 0.69 ±0.01eV at an irradiation fluence of \( 1 \times 10^{11} \) ions cm\(^{-2} \). After this fluence Schottky barrier height remains insensitive to irradiation upto the fluence value of \( 5 \times 10^{12} \) ions cm\(^{-2} \).

From the slope of \( \ln(I) \) versus \( V \) curve, the value of ideality factor is calculated using the relation

\[
n = \frac{q}{kT} \left( \frac{dV}{d \ln(I)} \right)
\]

(3.4)

The experimental value of ideality factor \( n \) derived from \( I-V \) data varies from 1.71 for unirradiated sample to 3.09 at irradiation fluence of \( 1 \times 10^{12} \) ions cm\(^{-2} \). The variation of ideality factor and Schottky barrier height as a function of irradiation fluence is shown in Figure 3.2.

The series resistance effect on the electrical characteristics of Au/n-Si Schottky structures and its dependency on irradiation fluence were investigated in the fluence range of \( 5 \times 10^9 \) ions cm\(^{-2} \) to \( 5 \times 10^{12} \) ions cm\(^{-2} \). The series resistance is a very important parameter of Schottky barrier devices. The resistance of the Schottky barrier device is the sum of total resistance value of the resistors in series and resistance in semiconductor device in the direction of current flow. The series resistance was evaluated from the forward bias \( I-V \) data using method developed
by Cheung et al [25]. The forward bias $I-V$ characteristics due to thermionic emission of a Schottky structure with the series resistance can be expressed as Cheung’s functions

$$\frac{dV}{d(ln I)} = IR_s + n\left(\frac{kT}{q}\right),$$ \hspace{1cm} (3.5)

$$H(I) = V - n\left(\frac{kT}{q}\right)\ln\left(\frac{I}{AA^*T^2}\right),$$ \hspace{1cm} (3.6)

and

$$H(I) = IR_s + n\Phi_s,$$ \hspace{1cm} (3.7)

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure3.2}
\caption{Irradiation fluence dependence of the Schottky barrier height and ideality factor for Au/n-Si Schottky structure.}
\end{figure}

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The term $IR_s$ is the voltage drop across the series resistance of Schottky diode. In Figures 3.3 (a) and 3.3 (b), experimental $dV/d(lnI)$ vs. $I$ and $H(I)$ vs. $I$ plots are presented at different ion fluences for Au/n-Si (100) Schottky barrier diode. Eq. (3.5) will give a straight line for the data of downward curvature region of $I-V$ characteristics. A plot of $dV/d(lnI)$ vs $I$ will give $R_s$ as the slope and $n(kT/q)$ as the y-axis intercept. As a function of irradiation fluence the values of ideality factor $n$, barrier height and series resistance $R_s$ derived from Figure 3.3 (a) and (b) are given in Table 3.1.

Using the $n$ value determined from Eq. (3.5), plots of $H(I)$ vs. $I$ will also give a straight line with y-axis intercept equal to $n\Phi_b$. The slope of these plots also provides a second determination of $R_s$, which can be used to check the consistency of this approach. Figure 3.4 shows the experimental series resistance values obtained from the semi-log forward bias $I-V$ characteristics as a function of irradiation fluence.

The most important characteristic of the metal-semiconductor (MS) interface is the nature of the potential barrier between the Fermi level in the metal and the majority carrier’s edge of the semiconductor at that interface. Since electrical contacts to semiconductors necessitate MS interfaces and depending upon this potential barrier height, interfaces exhibit a modest resistance to current flow in either direction or a low resistance to current flow in one direction and high resistance to current flow in the opposite direction [26]. The charge at MS interfaces can account for the difference between the predicted and the observed Schottky barrier height. It is more important to know how the barrier height varies with the applied voltage in the forward bias condition. The potential across the interface varies with bias because of the electric field present in the semiconductor and because of the change in
Figure 3.3: (a) Plots of $dV/d\ln(I)$ vs. $I$, and (b) $H(I)$ vs. $I$ for Au/n-Si(100) Schottky structure at different irradiation fluences.
Table 3.1: Irradiation fluence dependence of various parameters determined from forward bias I-V characteristics of Au/n-Si(100) Schottky structure

<table>
<thead>
<tr>
<th>Fluence (ions-cm$^{-2}$)</th>
<th>Ideality Factor ($n$)</th>
<th>Barrier Height (eV)</th>
<th>Resistance ($R_s$) from $dV/dln(I)$-I (Ω)</th>
<th>Resistance $H(I)$-I (Ω)</th>
<th>Density of interface states $N_{ss}$ (eV$^{-1}$cm$^2$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>1.71</td>
<td>0.74</td>
<td>3956</td>
<td>3992</td>
<td>4.71×10$^{12}$</td>
</tr>
<tr>
<td>5.0×10$^9$</td>
<td>1.60</td>
<td>0.73</td>
<td>4535</td>
<td>4542</td>
<td>4.00×10$^{12}$</td>
</tr>
<tr>
<td>1.0×10$^{10}$</td>
<td>1.57</td>
<td>0.73</td>
<td>5162</td>
<td>5203</td>
<td>3.85×10$^{12}$</td>
</tr>
<tr>
<td>2.5×10$^{10}$</td>
<td>1.89</td>
<td>0.71</td>
<td>6064</td>
<td>6172</td>
<td>6.15×10$^{12}$</td>
</tr>
<tr>
<td>5.0×10$^{10}$</td>
<td>2.32</td>
<td>0.70</td>
<td>6500</td>
<td>6550</td>
<td>9.06×10$^{12}$</td>
</tr>
<tr>
<td>7.5×10$^{10}$</td>
<td>2.70</td>
<td>0.69</td>
<td>5436</td>
<td>5602</td>
<td>1.16×10$^{13}$</td>
</tr>
<tr>
<td>1.0×10$^{11}$</td>
<td>3.08</td>
<td>0.69</td>
<td>4543</td>
<td>4634</td>
<td>1.40×10$^{13}$</td>
</tr>
<tr>
<td>2.5×10$^{11}$</td>
<td>3.09</td>
<td>0.69</td>
<td>4504</td>
<td>4543</td>
<td>1.43×10$^{13}$</td>
</tr>
<tr>
<td>5.0×10$^{11}$</td>
<td>3.09</td>
<td>0.69</td>
<td>4402</td>
<td>4348</td>
<td>1.43×10$^{13}$</td>
</tr>
<tr>
<td>1.0×10$^{12}$</td>
<td>3.17</td>
<td>0.69</td>
<td>4424</td>
<td>4216</td>
<td>1.43×10$^{13}$</td>
</tr>
<tr>
<td>5.0×10$^{12}$</td>
<td>3.20</td>
<td>0.69</td>
<td>4620</td>
<td>4560</td>
<td>1.43×10$^{13}$</td>
</tr>
</tbody>
</table>
Figure 3.4: variation of series resistance with irradiation fluence for Au/n-Si(100) Schottky structure

the interface states charge as a result of the applied voltage, and thus modifies the barrier height. The effective barrier height $\Phi_e$ is given by [27, 28]

$$\Phi_e = \Phi_b + \beta V = \Phi_b + \left(1 - \frac{1}{n(V)}\right)V$$

(3.8)

The $\Phi_e$ is assumed to be dependent on bias due to the presence of a native oxide interfacial layer and interface states located at the interfacial layer-semiconductor interface. $\beta$ is the voltage coefficient of the effective barrier height $\Phi_e$ and is a parameter that combines the effects of both the interface states and interfacial layer thickness for the cases in which
interface states are in equilibrium with the semiconductor. For the interface states in equilibrium with the semiconductor, the interface states density $N_{ss}$ is given by [24]

$$N_{ss} = \frac{1}{q} \left( \frac{\varepsilon_i}{\delta} \left( n - 1 \right) - \frac{\varepsilon_s}{W} \right)$$  \hspace{1cm} (3.9)

where $W$ is the space charge width, and $N_{ss}$ the density of interface states in equilibrium with the semiconductor, $\varepsilon_s$ and $\varepsilon_i$ are the permittivities of the semiconductor and the interfacial layer, respectively. $\delta$ is the thickness of the interfacial native oxide layer. The thickness of native oxide layer and depletion layer width can be obtained from high frequency $C-V$ measurements using the equations [22]

$$C_i = \frac{\varepsilon_i \varepsilon_0 A}{\delta}$$  \hspace{1cm} (3.10)

and

$$W_D = \sqrt{\frac{2 \varepsilon_s V_{bi}}{q N_D}}$$  \hspace{1cm} (3.11)

where $V_{bi}$ is the surface potential and $N_D$ is the dopant carrier concentration. Furthermore, in n-type semiconductors, the energy of the interface states $E_{ss}$ with respect to the bottom of the conduction band at the surface of semiconductor is given as

$$E_C - E_{ss} = q \Phi_e - qV$$  \hspace{1cm} (3.12)

The energy distribution or density curves of the interface states can be determined from experimental data of this region of the forward bias $I-V$ curves in Figure 3.1. Dependence of $N_{ss}$ converted to a function of $E_{ss}$ using Eq.(3.12) at various irradiation fluences is shown in Figure 3.5. For the as prepared sample the interface state density has an exponential rise (from $5\times10^{12}$ eV$^{-1}$cm$^{-2}$ in $E_C-0.68$ eV to $4.5\times10^{13}$ eV$^{-1}$cm$^{-2}$ in $E_C-0.56$eV) with bias from the mid-gap towards the bottom of conduction band.
Figure 3.5: The energy distribution profile of the interface state densities $N_{ss}$ obtained from the forward bias I-V characteristics of the Au/n-Si (100) Schottky structure at different irradiation fluencies.

The obtained values of interface states density are of the same order as reported in literature by some authors for Schottky structures [23, 29].

The density of interface states $N_{ss}$ increases with increasing irradiation fluence and after a fluence of $1 \times 10^{11}$ ions-cm$^{-2}$ remains almost constant, as the irradiation fluence increases further. The ideality factor shows the same trend with irradiation fluence as the interface states density. An increase in density of interface states results in a high value of ideality factor indicating dominance of other current transport mechanisms (field due to
emission, tunneling etc.) over the thermionic emission. These current mechanisms lead to an increase in leakage current value with increasing irradiation fluence as shown in Figure 3.1. After an irradiation fluence of $1 \times 10^{11}$ ions-cm$^{-2}$ leakage current also gets saturated. The Schottky barrier height decreases as the interface state density increases. When Schottky barrier diode is irradiated with a fluence of $5 \times 10^{10}$ ions cm$^{-2}$, the Schottky barrier height decreases to $0.70 \pm 0.01$ eV and as fluence increases to $1 \times 10^{11}$ ions cm$^{-2}$, the barrier height decreases to a value of $0.69 \pm 0.01$ eV and remains immune to irradiation fluence as fluence increases up to $5 \times 10^{12}$ ions-cm$^{-2}$. To understand the observed modifications in the Schottky barrier diode properties it is necessary to analyze the possible implications of ion transport through the sample. When $180$ MeV $^{107}$Ag$^{14+}$ ion passes through the metal- semiconductor interface, it loses energy via nuclear energy loss $S_n$ resulting from elastic collisions of the ion with the target atoms causing their displacement from the regular lattice sites, and electronic energy loss $S_e$ which induces ionization/excitation of electrons inside the solid. For $180$ MeV $^{107}$Ag$^{14+}$ ion, the variation of $S_n$ and $S_e$ as a function of depth inside the sample is shown in Figure 3.6. All the energy loss calculations were performed using standard Monte Carlo simulation program [30] called SRIM-2006. The ions stop deep inside the substrate far away from the MS interface. At the MS interface the $S_n$ value is $0.03$ keV/nm while $S_e$ is $12.6$ keV/nm (in the Si substrate). It is well established that $S_n$ causes creation of defects like vacancies, interstitials etc. at the interface [31] while $S_e$ produces strong ionization of the target atoms near the MS interface. During their relaxation, the electronic excitation can produce several specific structural defects and phase transition [32, 33] as well. These defects have their energy levels deep inside the semiconductor band gap and lead to an increase in the interface state density at the MS interface. These deep level defects trap the carriers and
Figure 3.6: The electronic and nuclear energy losses of 180 MeV $^{107}$Ag ions as a function of depth inside Au/n-Si (100) Schottky diode.

act as the scattering centers for the mobile carriers, hence, decreasing the carrier concentration and their mobility. This decrease in carrier concentration and mobility results in an increase in series resistance. Two theoretical models namely, thermal spike [34] and coulomb explosion [35] model are used to explain the local excitation of the lattice by energy transfer from the highly excited electronic system to the lattice atoms. Both mechanisms can result in atomic transport and swift heavy ions irradiation of solids leads to materials modification depending on the properties of the materials and deposited energy density [36,
According to the widely used thermal spike model, rapid energy transfer through electron phonon coupling makes the system highly excited and the region around the ion track gets suddenly heated to a very high temperature within small time duration [38]. Therefore, a lot of vacancies are produced everywhere along the ion track. The numbers of vacancies generated are of the order of \(10^{19}\) cm\(^{-3}\), which have a typical diffusion length of 25 nm in Si [39, 40]. At the lower fluences, the resistance increases because the number of vacancies increases as the irradiation fluence increases. At an irradiation fluence of \(5 \times 10^{10}\) ions-cm\(^{-2}\) the defect regions around the ion tracks cover the whole area and produce maximum vacancies and interstitials. After these fluences, defect regions around the tracks start overlapping. The decrease in the value of resistance after fluence \(5 \times 10^{10}\) ions-cm\(^{-2}\) indicates that product of the mobility and the free carrier concentration has increased.

Figure 3.7: Reverse bias capacitance-voltage characteristics of Au/n-Si (100) Schottky diode at different ion irradiation fluences.
From $C-V$ characteristics shown in Figure 3.7, it is found that carrier concentration is decreased with increasing irradiation fluence. From the slope of the curves, carrier concentration have been calculated using Eq.(2.21) of Chapter 2. Carrier concentration decreased from a value of $5 \times 10^{15}$ cm$^{-3}$ for unirradiated diode to $1.2 \times 10^{15}$ cm$^{-3}$ after irradiation at a fluence of $5 \times 10^{12}$ ions-cm$^{-2}$. It implies an increase in the mobility, which may be due to the migration of vacancies and recombination of vacancy-interstitials. Recently, it is has been observed that swift heavy ion irradiation results in annealing of point defects due to electronic energy loss when a amorphous Si wafer was irradiated with 100 MeV Ag$^{7+}$ ion beam [41]. It is evident from Figure 3.6 that at the MS interface $S_e$ value is about 350 times larger than $S_n$. This high value of $S_e$ may cause partial annealing of point defects produced by $S_n$. So the cumulative effects of $S_n$ and $S_e$ result in constancy of interface state density. This constancy of interface states leads to immunity of diode parameters with respect to fluence. After the irradiation fluence of $1 \times 10^{11}$ ions cm$^{-2}$ the Schottky barrier height, ideality factor, and series resistance remain almost constant upto a fluence $5 \times 10^{12}$ ions cm$^{-2}$. These results suggests that after fluence of $1 \times 10^{11}$ ions-cm$^{-2}$ rate of creation of defects and rate of annealing of defects become equal resulting in constancy of interface state density as well as Schottky barrier parameters with respect to irradiation in the range from $1 \times 10^{11}$ ions-cm$^{-2}$ to $5 \times 10^{12}$ ions-cm$^{-2}$.

3.3.2 Temperature-dependent barrier characteristics of swift heavy ion irradiated Au/n-Si Schottky structure

3.3.2.1. Capacitance-voltage characteristics

The $C-V$ characteristics have been analyzed using the Schottky-Mott equation [22]

$$C = \varepsilon_S A \frac{W}{W} = \sqrt{\frac{q \varepsilon_S N_D A^2}{2(V_{bi} - V - V_T)}}$$  \hspace{1cm} (3.13)
where \( \varepsilon_s \) is the dielectric constant of the semiconductor, \( A \) is the area of the Schottky diode, \( W \) is the depletion width, \( N_D \) is the concentration of ionized donor atoms, \( V_{bi} \) is the built-in potential, \( V_T (= kT/q) \) is the thermal voltage and \( V \) is the applied reverse bias. Using Eq. (3.13) the value of \( N_D \) can be written as

\[
N_D = \frac{2}{q\varepsilon_s} \left[ \frac{-1}{d\left(\frac{A^2}{C^2}\right)/dV} \right].
\]

(3.14)

Hence from the slope of \( 1/C^2 \) versus \( V \) curve the value of ionized dopant concentration \( N_D \) or free carrier concentration can be obtained. The Schottky barrier height \( \Phi_B(C-V) \) is related to the built-in voltage \( V_{bi} \) by the following equation

\[
\Phi_B(C-V) = V_{bi} + \frac{kT}{q} \ln \left( \frac{N_c}{N_D} \right)
\]

(3.15)

with

\[
N_c = 2\left(\frac{2m^*kT}{\hbar^2}\right)^{3/2}
\]

(3.16)

where \( N_c \) is the effective density of states in Si conduction band, \( m^* = 1.08 \, m_0 \) is the effective mass of electrons in Si and \( m_0 \) is the rest mass of electron [22]. From the intercept of the \( 1/C^2 \) versus \( V \) curve on the voltage axis, the value of \( V_{bi} \) is calculated.

Figure 3.8 shows the \( 1/C^2 \) versus \( V \) characteristics of irradiated (fluence \( 5 \times 10^{11} \) ions-cm\(^2\)) Au/n-Si Schottky diode at different temperatures. The capacitance decreases as a function of temperature. At room temperature the value of capacitance at zero bias was 255 pF while at a temperature 50K its value decreased to 195 pF. From the experimental \( 1/C^2 \) versus \( V \) curve, the values of donor concentration \( N_D \) and Schottky barrier height \( \Phi_B(C-V) \) have been determined. The donor concentration at room temperature was \( 1.27 \times 10^{15} \) cm\(^{-3}\). It then decreased with decrease in temperature and at a temperature of 50K its value reduced
to $1.07 \times 10^{15}$ cm$^{-3}$. The value of Schottky barrier height for irradiated diode at 300K was 0.86 eV and then it increased with decreasing temperature. At a temperature of 50K, the value of Schottky barrier height increased to 0.90 eV. The variation of Schottky barrier height with temperature is shown in Figure 3.9.

The observed modification in the $C$-$V$ characteristics has been understood in framework of implications of high-energy ion irradiation at the MS interface. As discussed in section 3.3.1, swift heavy ion transfers its energy to the solid by mainly two mechanisms: (1)

**Figure 3.8:** Reverse bias Capacitance-voltage characteristics of irradiated Au/n-Si(100) Schottky barrier diode at different temperatures.
Figure 3.9: Temperature dependence of the zero-bias barrier height, flat-band barrier height and C-V barrier height for the irradiated Au/n-Si(100) Schottky barrier diode.

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 [42, 43]. The elastic collision creates the defects in semiconductor material like vacancies and interstitials. Combination or agglomeration of these defects leads the formation of complex and stable defect structures [31, 32, 44]. These defects have associated deep levels present inside the band gap of silicon and they act as traps for the free carriers resulting in reduction of their concentration. The swift heavy ion irradiation of silicon produces traps levels at $E_C - 0.23$ eV, and $E_C - 0.43$ eV, which belongs to vacancies and their combinations [45, 46] while the energy levels at $E_C - 0.62$ eV and $E_C - 0.86$ eV belongs to interstitial point defects and clusters [47-51]. The decrease in capacitance of the Schottky diode implies a widening in the semiconductor
depletion width. Since the charge neutrality condition at the interface should be satisfied, widening of the depletion width results from a reduction of the ionized donor concentration. One of the possible mechanisms causing a decrease in the net ionized donor concentration is the presence of negatively charged deep defect centers which has been shown by researchers using DLTS measurements [32, 44]. The presence of these levels causes a drop in the capacitance at lower temperature. This is confirmed from the experimental C-V characteristics. This behavior is due to a freeze out of electrons on the deep centers in the band gap and causes a strong increase in the series resistance of the diode, which makes the measured capacitance to appear smaller. The presence of these centers causes the compensation of the positive shallow donors in the depletion region so that the effective net ionized-donor concentration is decreased. The donor compensation results in widening of the depletion width so that the charge-neutrality condition is maintained at the MS interface. As can be seen from Eq.(3.13) the increase in the depletion width results in decrease in Schottky diode capacitance.

3.2.3.2. Current-voltage characteristics

The temperature dependent I-V curves were fitted to the thermionic emission equation (3.1). Figure 3.10 shows the ln(I) versus V characteristics of Au/n-Si diode at different temperatures. The values of ideality factor $n$ and Schottky barrier height $\Phi_B$ of the diode are calculated using the Eq.(3.3) and Eq.(3.4). These values are plotted as a function of temperature in Figure 3.11. The ideality factor $n$ exhibits an increasing trend with decreasing temperature, whereas the Schottky barrier height decreases with decreasing temperature.
Figure 3.10: Temperature dependent $\ln I$ vs $V$ characteristics of irradiated Au/n-Si(100) Schottky barrier diode.

Usually, the forward bias $\ln(I)$ versus $V$ characteristics are linear at low forward bias voltages, but deviate considerably from linearity due to the effect of series resistance, the interfacial layer and the interface states when the applied voltage is sufficient large. The series resistance is significant in downward curvature of forward bias $\ln(I)$-$V$ characteristics, but the other two parameters are significant in both the linear and non-linear regions of $\ln(I)$-$V$ characteristics. The lower the interface state density and series resistance, the greater the range over which $\ln(I)$-$V$ curve yields at straight line [52]. As the linear range of the forward $\ln(I)$-$V$ plots is reduced, the accuracy of the determination of $n$ and $\Phi_B$ becomes poorer. The barrier height of a Schottky barrier depends on the electric field across the contact and
consequently on the applied bias voltage. Therefore, it is necessary to specify standard field conditions. The electric field in the semiconductor is zero under flat-band conditions, which eliminates the effect of tunneling and image force lowering from affecting the $I-V$ characteristics. The barrier height obtained under the flat-band conditions is called flat-band barrier height. Flat-band barrier height is the real barrier height which should be used when comparing experiments with theory [53, 54]. In order to obtain the flat-band barrier height, the analysis of Wagner et al [53] and Chin et al [54] have been followed. The flat band barrier height is given by

$$
\Phi_{bf} = n\Phi_B(I-V)-(n-1)\frac{kT}{q} \ln \left( \frac{N_C}{N_D} \right)
$$

(3.17)

where $N_C$ and $N_D$ are functions of temperature. The experimental carrier concentrations $N_D$ depending on the temperature are calculated from the reverse bias $I/C^2$ versus $V$ plots in Fig 3.8. The values of $N_C$ and $N_D$ are $2.8 \times 10^{19}$ cm$^{-3}$ and $1.21 \times 10^{15}$ cm$^{-3}$ at 300K, which become $1.91 \times 10^{18}$ cm$^{-3}$ and $1.08 \times 10^{15}$ cm$^{-3}$ at 50K, respectively. The flat-band barrier height is calculated from zero-bias $I-V$ barrier heights and corresponding ideality factor at each temperature. Figure 3.9 shows the variation of the flat-band barrier height $\Phi_{bf}$ as a function of the temperature. The flat-band barrier height is invariably larger than the zero-bias barrier height at low temperature.

From the Figure 3.9, it can be seen that the flat-band barrier height is essentially the same as the barrier height determined by the capacitance-voltage ($C-V$) method. Flat-band barrier height measurements are in good agreement between the values of barrier height obtained from both methods over a wide temperature range. The temperature dependence of the flat-band barrier height in the range 50-300 K can be expressed as
\[ \Phi_{bf}(T) = \Phi_{bf}(T=0K) + \alpha T \]  

(3.18)

where \( \Phi_{bf}(T=0K) \) is the flat band barrier height extrapolated to zero temperature and \( \alpha \) is temperature coefficient of the barrier height. The fit of Eq.(3.18) to the data shown in Figure 3.9 gives \( \alpha = -7.4 \times 10^{-6} \text{ eVK}^{-1} \) and \( \Phi_{bf}(T=0K) = 0.88 \text{ eV} \) respectively. This low value of temperature coefficient implies that the Fermi level is pinned by interface defects or imperfections at the MS interface. If defects caused the Fermi level pinning, the temperature change of the barrier would reflect the temperature motion of the defect relative to the appropriate band edge i.e. their ionization entropy. Revva et al [15] pointed out that if the

![Graph showing temperature dependence of ideality factor and zero bias barrier height.](image)

**Figure 3.11:** Temperature dependence of the ideality factor and zero bias barrier height for the irradiated Au/n-Si(100) Schottky barrier diodes in the temperature range of 50-300K.
Fermi level is pinned by the defects, the barrier height of an n-type semiconductor changes only weakly with temperature because their ionization entropy changes only weakly with temperature. This explains the results obtained for the irradiated Schottky contact. Earlier studies [45-51] on the irradiation of Si reported that the divacancy, impurity-vacancy combinations and interstitial defect clusters are the radiation induced defect centers in silicon. The irradiation of Si give rise to a trap level at 0.27±0.02 eV above the valence band maximum due to interstitial point defect clusters [47-51]. Pinning of the Fermi level at this energy results in a barrier height of 0.85±0.02 eV, which is in close agreement with the barrier height measured for irradiated Au/n-Si Schottky diodes. In conclusion, the defects at the interface (deep levels) are responsible for the weak temperature dependence of the barrier height for Au/n-Si(100) contacts.
3.3 CONCLUSIONS

In this chapter the results of *in situ* $I$-$V$ and $C$-$V$ measurements on Au/n-Si (100) Schottky diodes are presented and discussed. It is found that Au/n-Si Schottky diode characteristics are very sensitive at lower irradiation fluences, the Schottky barrier height decreases while the ideality factor, series resistance, leakage current and interface states density increases as the ion fluence increases. After a critical fluence diode parameters remains nearly constant with irradiation fluence. The Schottky diode parameters are influenced by the density of interface states. The cumulative effects of large electronic energy loss and nuclear energy loss at the MS interface have been used to explain the observed behavior. When annealing of defects balances the rate of creation of defects, constancy in the diode parameters with respect to irradiation fluence occurs. The $C$-$V$ and $I$-$V$ measurements have been made in the temperature range of 50-100K to investigate the barrier characteristics of the irradiated Au/n-Si (100) Schottky barrier diode and discussed. The ideality factor and zero-bias barrier height are found to be strong functions of temperature while the flat-band barrier height is almost independent of the temperature. The negligible temperature dependence of the flat-band barrier height suggests that the interface defects produced by the high energy heavy ion irradiation are responsible for the pinning of the Fermi level because their ionization entropy is only weakly dependent on the temperature. It is found that the barrier heights obtained by $I$-$V$ measurements are in close agreement with the barrier height found by $C$-$V$ measurements at 1MHz.
References


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