Chapter - 4

METAL-SEMICONDUCTOR INTERFACE: THE SCHOTTKY DIODE

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4.1 Introduction to the Schottky Diode

In 1938, Walter Schottky, the son of German mathematician Friedrich Schottky, explained the manner in which a specific combination of a metal and a doped semiconductor material can rectify current conduction. From then onward, the Schottky diode became a key element in designing various electronics circuits. Rectification in Schottky diodes occurs because of the difference in work function between the metal and the semiconductor. Conduction is controlled by thermionic emission of majority carriers over the barrier created by the unequal work function of different materials. The Schottky diode is therefore, a majority carrier device whose switching speed is not limited by minority carrier effects [79]. Therefore, this diode can cease current conduction faster than an ordinary diode. This property allows for a smaller diode area and faster transitions. These properties make it ideal for many Radio-Frequency applications [80]. In addition, these devices have a low forward voltage drop, and a lower power loss takes place than in any ordinary silicon pn-junction diodes. This enhances the demand of Schottky diodes in power device applications [81].

Current-Voltage (I-V) and Capacitance-Voltage (C-V) characteristics of a metal-semiconductor interface give enormous depths of information of physical and electrical properties of a bulk semiconductor material and its surface [2]. Therefore, to understand Gallium Antimonide (GaSb) as a material, the Schottky diode was chosen as a vehicle for the investigation. However, achieving an ideal rectifying contact for GaSb is much more difficult than it is for Silicon (Si) or Gallium Arsenide (GaAs) because of the oxidation of the GaSb surface. Furthermore, while several researchers have fabricated Schottky diode on n-GaSb, Schottky diodes on p-GaSb have hitherto not been prepared. This is because p-GaSb Schottky diodes are, by nature, almost ohmic in resistance. Therefore, it is difficult to carry out reliable current-voltage or capacitance-voltage measurements in case of Schottky diodes using p-GaSb. Besides this problem, GaSb is a narrow band gap material. Hence, achieving high quality metal-GaSb Schottky diode with ideal current-voltage characteristics is very difficult. Above all, interface properties like existence of interfacial layers, and the presence of high defect densities at the surface of the metal-semiconductor interface lead to non-ideal characteristics [2, 6, 82-90]. Due to all these detrimental issues it seems very challenging to grow such a compound and make rectifying contacts on it. Therefore, a simulation was carried out prior to the fabrication to study the ideal behaviour of the Schottky diode using SILVACO TCAD tool [69]. In the ideal metal-semiconductor interface, the charge carriers should not encounter any kind of resistance, whereas, in reality contact resistance also exists and this contact resistance manifests in a resulting barrier potential which is non-ideal [7].

Various metals have been used to fabricate Schottky diodes on n-GaSb. The barrier heights of fabricated Schottky diodes with gold, nickel and silver metal deposition on vacuum cleaved GaSb substrate have been reported to be 0.64-0.84 eV, 0.43-0.46 eV and 0.38-0.44eV respectively [91-93]. Even though the Schottky barrier height lies within a small range of values from 0.5eV to 0.6eV, it mainly depends on the fabrication technique. As is well known, irrespective of the fabrication technique used, GaSb is always p-type in nature. Thus, the bulk GaSb grown by us using the VDS method was also p-type in nature. However, for fabrication of Schottky diodes n-GaSb substrates are needed. Therefore, we have used Tellurium-doped GaSb to fabricate a Au/n-GaSbSchottky diode for the metal-semiconductor interface study.

The systematic investigation carried out is described in three sections:

- Theoretical study on the transport mechanism of Schottky diodes,
- Detailed investigation of interface properties of the metal-semiconductor interface of Au/n-GaSb Schottky diode using SILVACO TCAD tool,
- Comparison of the simulated result with the results of the experimentally fabricated Au/n-GaSb Schottky diode to validate the authenticity of the simulation model and the material properties used.

4.2 Theory of the Schottky diode

The metal/semiconductor contact is a simple and important device among the semiconductor devices family. The performance of a Schottky diode is determined by the properties of the barrier of the contact interface. The quality of the barrier is evaluated by the Schottky barrier height and ideality factor, η. For an ideal case of a Schottky barrier, the barrier height is simply the difference between the metal work function and the election affinity of the semiconductor, and the η is usually taken as 1. The forward bias current transport mechanism of a Schottky diode obeys the thermionic emission principle when the applied voltage (V) is more than 3KT/q. The thermionic current can be written from [2,3] as

$$I = I_0 \exp\left(\frac{qV}{\eta kT}\right)\left[1 - \exp\left(-\frac{qV}{kT}\right)\right] \tag{4.1}$$

Where I_0 is the reverse saturation current density and defined as

$$I_0 = A^{**}T^2 \exp\left(-\frac{q\,\phi_B}{kT}\right) \tag{4.2}$$

Where A^{**} is the effective Richardson constant and Φ_B is the barrier height of the Schottky diode and η is called ideality factor and written in the form of

$$\eta = \left(\frac{q}{KT}\right)\frac{d(V)}{d(lnI)} \tag{4.3}$$

By plotting equation (4.3) between Ln I and the forward voltage the Y-intercept gives the reverse saturation current I_0 and from the slope of the plot the η can be obtained. In addition, the barrier height (Φ_B) can be determined from equation (4.2). But instead, we have determined the barrier height (Φ_B) of the diode from another technique called the high frequency (1MHz) capacitance-voltage characteristics using the equation (4.4):

$$\Phi_B = V_{diff} + \Phi_{fn} + KT/q \tag{4.4}$$

Where V_{diff} is the voltage intercept at $1/C^2=0$ and Φ_{fn} is the potential difference between the Fermi level and the conduction band edge. V_{diff} has been determined from the voltage versus inverse C^2 plot from the data of C-V characteristic. In a practical Schottky diode, the I–V characteristics of the metal/semiconductor contacts usually deviate from the ideal thermionic emission (TE) current model.

4.3 Fabrication of Au/n-GaSb Schottky Diode

For fabrication of Au/n-GaSb Schottky diode, a Tellurium-doped GaSb wafer was used. The wafer was obtained from an ingot of 2.5 cm length and 0.8 cm diameter

Tellurium-doped GaSb sample grown using the Vertical Bridgeman method [94]. The sample wafer was cut perpendicular to the ingot axis by a diamond saw cutter. One side of the wafer was polished mechanically to a mirror-finish surface. The sample was found to be n-type from the Hall Effect study. A rectangular (0.5 cm X 0.5 cm) sample piece was cut from the wafer and then quickly put inside the vacuum coating chamber and the chamber was evacuated. High purity gold was then thermally evaporated onto it through a metal mask under a vacuum of 10^{-6} torr. The diameter of the Schottky diode was 0.1cm. Ohmic contact was made by melting a high purity indium metal dot of 0.1cm diameter on the back side of the sample. The metallisation was carefully performed in a reducing atmosphere (1% Hydrogen in Argon) to avoid oxygen contamination. The ohmic contact was verified from the I-V characteristics. The Schottky diode fabricated was characterised through current-voltage and capacitance-voltage measurements (1MHz) using NI PXI-4072 of National Instruments. All the measurements were performed at room temperature.

4.4 Simulation Model of a Schottky Diode

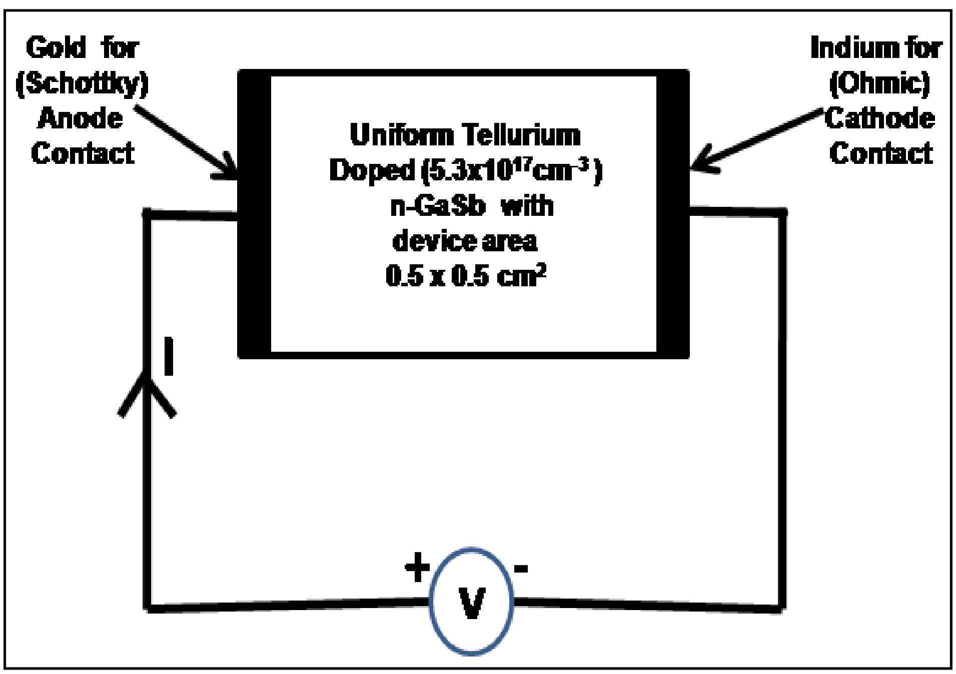

Figure 4.1. Structure and Sign Convention of the Simulated Schottky Diode

The simulated structure corresponding to the experimental Schottky diode under test is shown in Figure 4.1. Material properties like band gap, permittivity, saturation mobility and carrier life time data at room temperature were taken from literature [6, 96].

Appropriate models like fldmob, bgn and srh of SILVACO TCAD tool were used to take care of the physics of metal-semiconductor interface [69]. The area and doping density of the simulated Schottky diode was kept the same as that of the experimentally fabricated diode. As it is well known that undoped bulk GaSb is always p-type in nature [6, 96], hence, to match the experimental sample, the simulated GaSb substrate has been converted from p-type to n-type by uniformly doping by tellurium to a doping density of 5.3 x 10^{17} cm^{-3}. Thereafter, at one side of the GaSb substrate anode contact is made with gold film to realize Schottky diode and the opposite side of the GaSb substrate is further doped by tellurium with the concentration of $1.4x10^{20}$ cm^{-3} to make the cathode Ohmic contact to make series resistance (R_s) insignificant. To characterize the I-V analysis, a DC potential is applied and current at room temperature were calculated. Later the CV curves were obtained and analysed by applying a small AC voltage from 10 Hz – 1 MHz in steps. Thereafter, the electrical properties of the Schottky diode, like the barrier height (φ_B) and ideality factor (η), were obtained and compared with that of the experimental results.

4.5 Results and Discussion

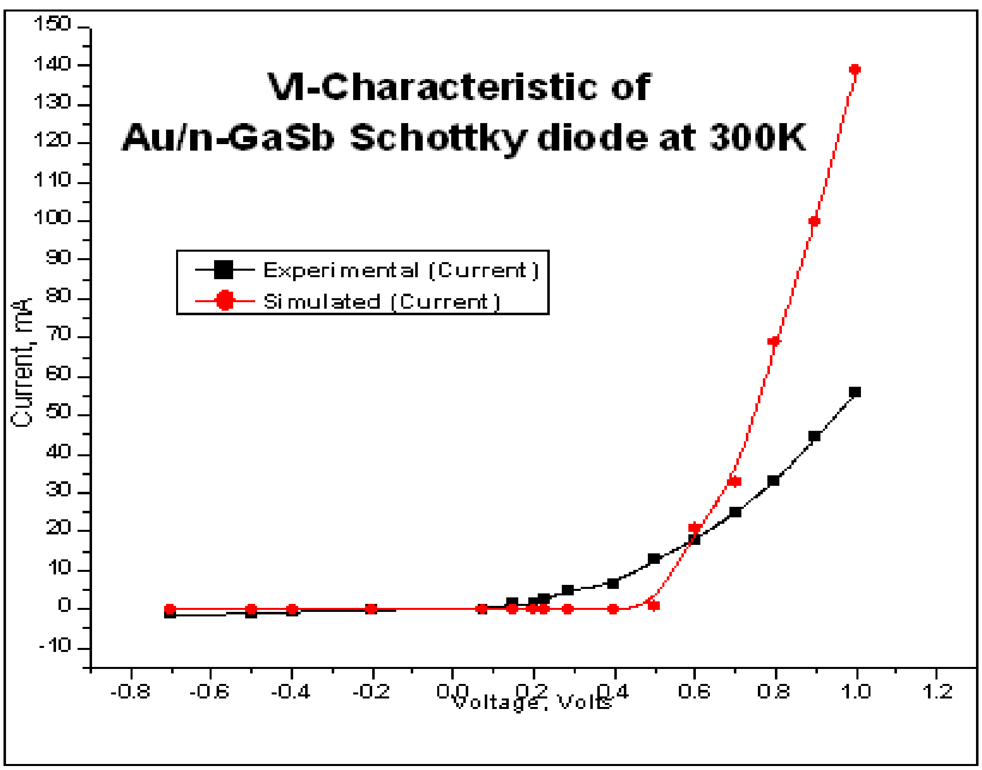

Figure 4.2. Current and Voltage Characteristics of Au/n-GaSb Schottky Diode Fabricated and Simulated at 300K

The typical Current-Voltage characteristics of both the Schottky diode fabricated experimentally and that of the model simulated using the TCAD tool are shown in Figure 4.2. It is observed that both the reverse and forward currents are found higher for the simulated contact as compared to that of the fabricated Schottky diode. The decrease in current in case of the fabricated structure may be due to the non-idealities present like the existence of interfacial layers and the presence of high defect densities at the surface of the fabricated structure. The reverse current of the Schottky barrier is governed either by tunnelling through mid-gap and surface leakage or by band-to-band tunnelling at higher voltages [6].

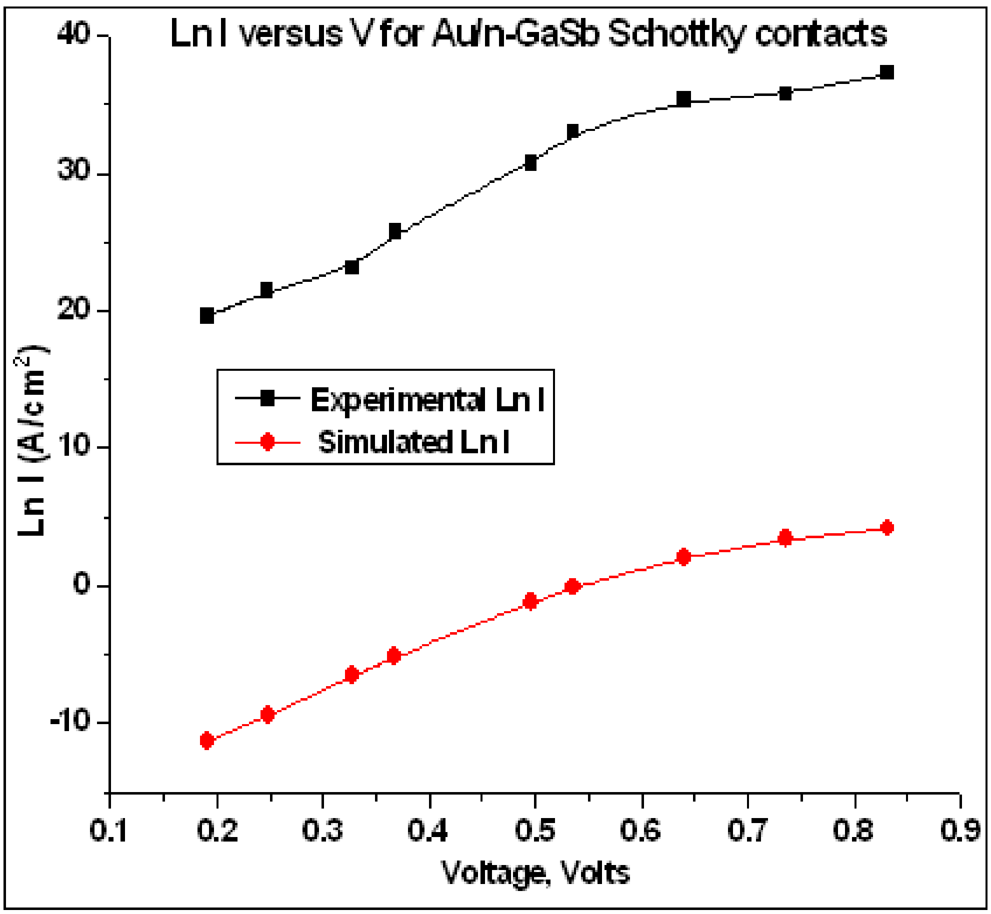

Figure 4.3. Current and Voltage Characteristics of Au/n-GaSb Schottky Diode Fabricated and Simulated at 300 K

The ideality factor and barrier height for both the diodes were calculated from the slope and intercept of the ln I v/s V plots as shown in Figure 4.3 using Equations from (4.1) to Equation (4.3). The corresponding values were found to be 2.1 and 0.48 eV for the fabricated Schottky diode whereas for the simulated structure they were 1.4 and 0.56 eV respectively. The ideality factor of diodes usually varies in the range of 1.3-2.4. The high value of the ideality factor is due to the generation-recombination current from a near mid-gap center [6]. From the analysis of the I-V data, the lower value of the barrier height (Φ_B) of the fabricated contact with respect to simulated contact may be because of the heavy doping effect in the semiconductor. Since the substrate taken is of a degenerated type; therefore, the tunnelling current, in addition to the thermionic current, leads to a higher value of I_S. This is because the experimentally determined ideality factor is larger than the ideality factor determined from simulation, resulting in a reduction in Φ_B. Furthermore, the current transport mechanism in GaSb involves electrons from the central Γ valley of the conduction band. Since the separation of the Γ valley and L valley is very small (~0.02eV), the transport is dominated by electrons occupying states in the L valley. Thus, the effective Richardson constant has to be higher than the value considered due to higher effective mass of the L valley electrons [6, 96].

The ideality factor is the measuring parameter of any diode which explains how accurately it follows the ideal diode characteristic equation. For an ideal contact, η should be equal to unity, but while the device was fabricated, the η deviates from the ideal ideality due to the interfacial layer between the semiconductor and the metal. Another possibility of higher value of experimentally found ideality factor (i.e. $\eta = 2.1$), can also be explained as due to tunnelling in heavily doped semiconductors. The deviated values of η obtained from simulation results were found out from the linear part of the simulated I-V curves. To obtain the non-ideal value of η from the simulation results, the linear part of I-V characteristic has been analysed with the assumptions that the thermionic-emission-diffusion is predominant and the existence of series resistance is neglected. The calculated value of η is found to be 1.4 at 300K, which is close to the reported value of 1.14 [97]. Furthermore, the ideality factor shows strong temperature dependence by decreasing smoothly from 1.096 to 2.3 as the temperature increases from 30K to140K, as depicted in Figure 4.4.

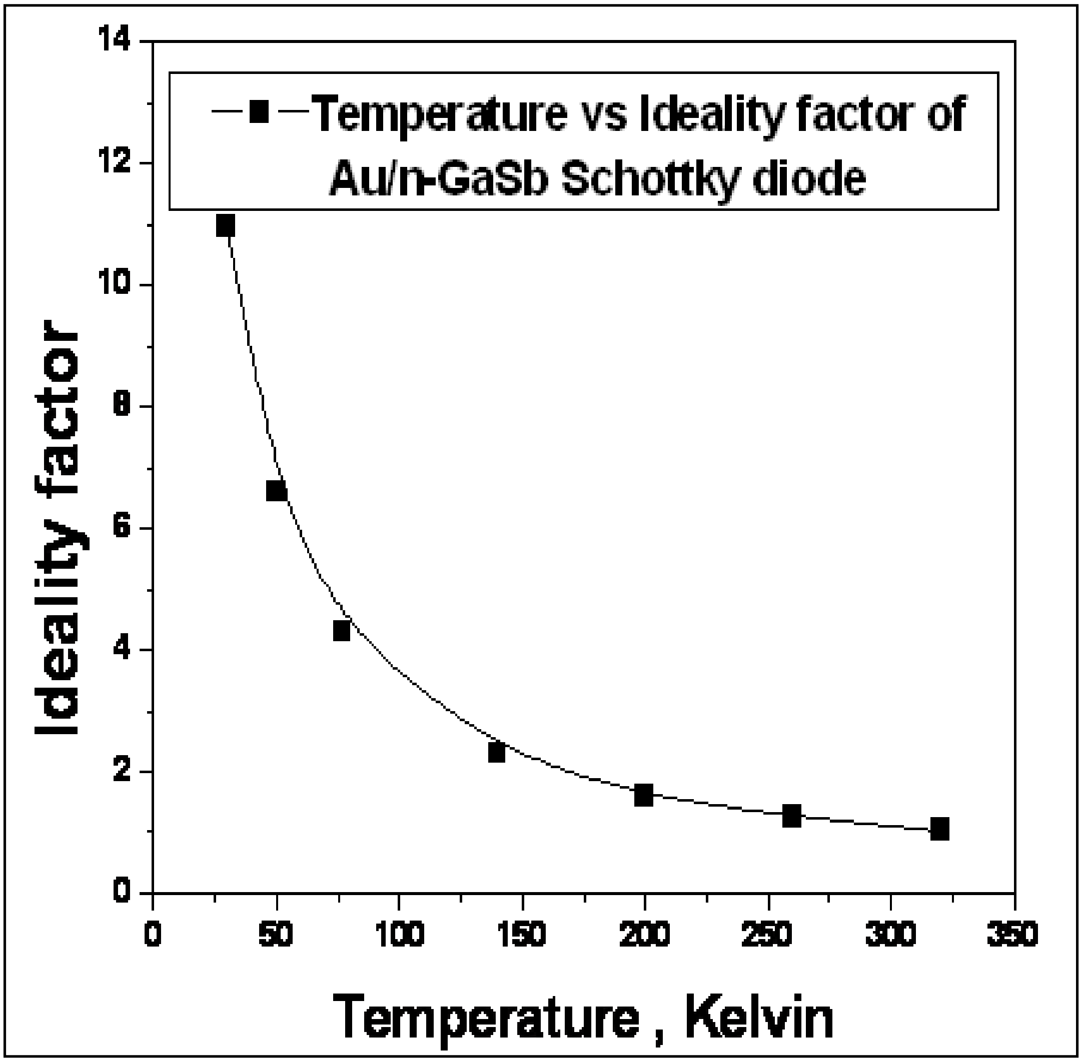

Figure 4.4. Simulated Result of Temperature v/s Ideality Factor in a Tellurium-doped Au/n-GaSb Schottky Diode

The barrier height found from the I-V characteristic increases from 0.11eV to 0.56 eV when temperature increases from 30K to 300K. The calculated Φ_B from the simulated I-V characteristic for various temperatures is shown in Figure 4.5. These results are similar to the reported temperature dependence of $\Phi_{B,}$. Furthermore, literature also reports that Φ_B for a Au-Schottky barrier on GaSb increases more or less linearly with increasing temperature (with a temperature coefficient of $-0.3\text{x}10^{-4}$eV/K) [98].

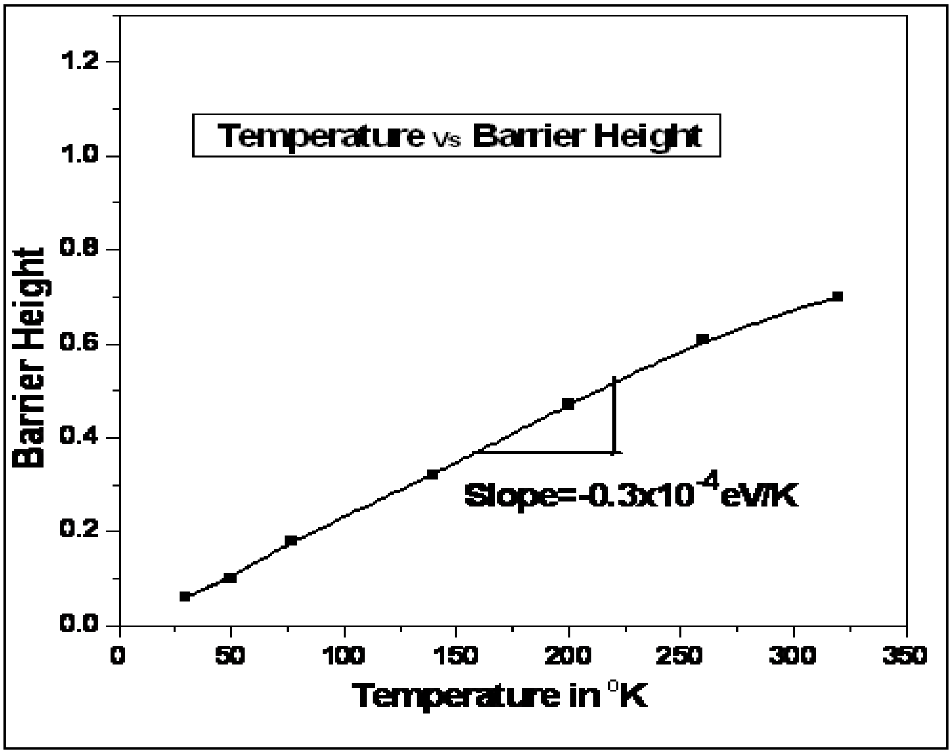

Figure 4.5. Simulated Results of Temperature v/s Barrier Height of a Tellurium-doped Au/n-GaSb Schottky Diode

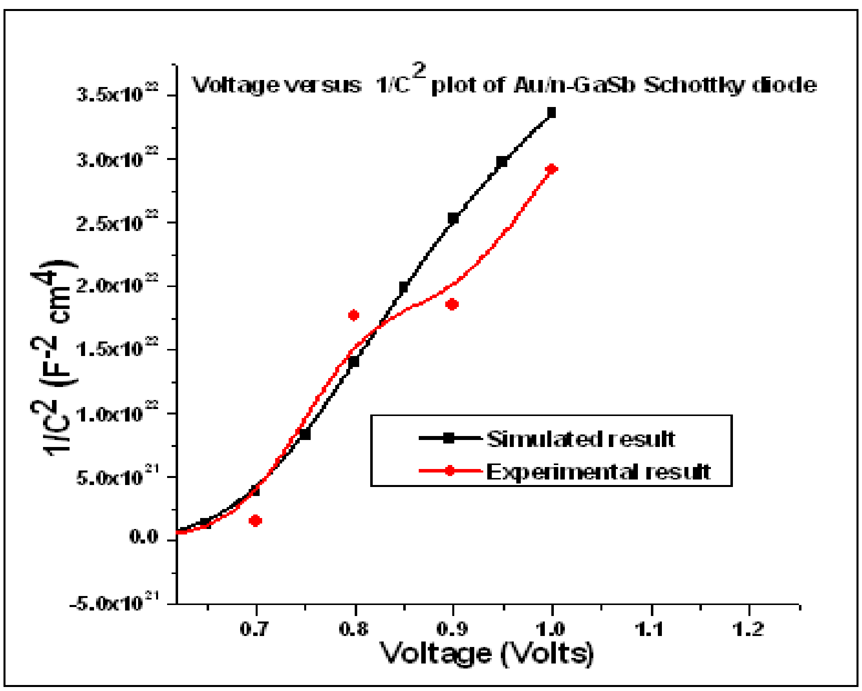

Figure 4.6. Voltage vs $1/C^2$ plot of Au/n-GaSb Schottky Diode Fabricated Experimentally and Simulated at 300K

The barrier height was also determined from the intercept at the voltage axis of the inverse C^2-V plot as shown in the Figure 4.6. The non-linearity of the inverse C^2-V plot was observed at lower voltages, which indicates the presence of deep levels in the forbidden gap of the substrate [2]. The barrier height values found for the contacts experimentally fabricated and of the simulated structure were to be 0.64 ± 0.01 eV and 0.7 eV respectively. The barrier heights, determined from the forward I-V characteristics, were found to be lower than the value obtained experimentally from the inverse C^2-V plot for the contacts and the simulated structure and were analysed in Table 4.1. The lower value of Φ_B deduced from the forward I-V characteristics might be due to the image force lowering of the barrier height whereas the value obtained from the capacitance measurement is not affected by image force as has been explained by Chang and Sze [99].

Table 4.1. A Comparative Study of Schottky Parameters Found from I-V and C-V Characteristics for Fabricated and Simulated Au/n-GaSb Schottky Diodes at 300K

Extracted From / Structure	I-V Characteristics				C-V Characteristics	
Schottky Contact	**Ideality Factor (η)**	**Reverse Saturation Current (I_0) (A/cm^2)**	**Resistance (R) (Ω)**	**Barrier Height (ϕ_B) (eV)**	**Barrier Height (ϕ_B) (eV)**	**Doping Density (N_D) (cm^{-3})**
Fabricated	2.1	4.3×10^{-3}	15.2	0.48	0.64	5.3×10^{17}
Simulated	1.4	2.56×10^{-16}	0.009	0.56	0.7	6.45×10^{17}

The presence of surface states may also be responsible for the low value of Φ_B obtained from the I-V curve. Furthermore, the significant decrease in the barrier height Φ_B may be due to the increased ideality factor due to high doping concentrations. The series resistance of the contact simulated was found to be ~ 0.009 ohms, whereas that of the fabricated contact was found to be ~ 15 ohms. The higher value of series resistance of the fabricated Schottky diode is due to non-idealities like dangling bonds and segregation impurities. The lower the series resistance the higher is the I_S, which in turn may bring down the barrier height and increase the ideality factor, since the tunnelling effect becomes dominant.

4.6 Chapter Summary

In this chapter, a preliminary investigation has been made to obtain the physical and electrical properties of Au/n-GaSb Schottky diode. Current-Voltage (I-V) and Capacitance-Voltage (C-V) is chosen as a vehicle to investigate the Schottky diode electrical properties. The barrier height and ideality factor were found both of the experimentally fabricated contact and of the simulated structure, and then compared for validation. At room-temperature, the barrier height of the Au/n-GaSb Schottky diode, found from the simulated structure, were 0.56 eV from I-V and 0.7 eV from C-V which are close to the precisely reported experimental results 0.64 eV. It is interesting to note that the barrier height determined from the I-V characteristic is a simple and direct method, but the barrier height obtained from the C-V characteristic is more reliable and consistent. This is probably because the I-V method is based upon forward bias condition with high current passing through the Schottky diode whereas the C-V method is based upon reverse bias conditions and contributes reverse leakage current. Apart from the barrier height parameter, the simulated ideality factor at 300K comes out to be 1.03, which is close to experimental value 1.4. In addition to this barrier height and ideality factor found for the simulated Au/n-GasbSchottky diode for a temperature range of 30K-300K shows that with the increase of temperature, barrier height increases whereas ideality factor decreases and shows good agreement with the reported values.