EE532: Device Simulation Lab

Experiment No. 4

Name: PRIKSHAT SHARMA
Entry No: 2023EEM1023
September 27, 2024

Experiment Name: Design and analysis of the MS contact and Schottky Diode(n-type) using Sentaurus TCAD.

1 Design Parameters

Table 1: Design Parameters

Substrate	Silicon
N-type Dopant with concentration	Phosphorous ($5 \times 10^{16}/cm^3$)
Doping type	Constant profile placement
Gate metal	Aluminium
Metal thickness	40nm
Metal work-function	4.0eV,4.3eV

2 Physics Models

Table 2: Physics Models

Parameters	Value/Type
Band gap and Bandgap narrowing	Effective intrinsic density (no band gap narrowing)
Mobility models	Mobility (Doping Dependence High Field Saturation)
Temperature (K)	300K

3 Device Structure

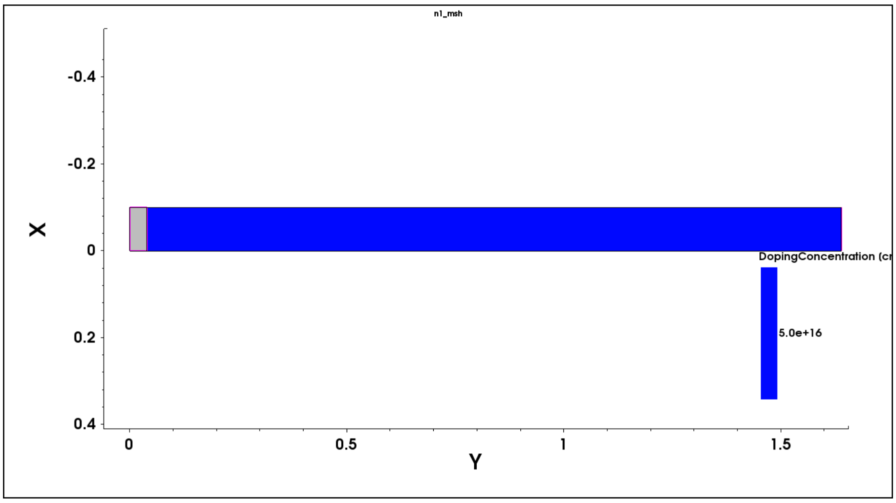

Figure 1: Schematic of the MS contact/Schottky Diode

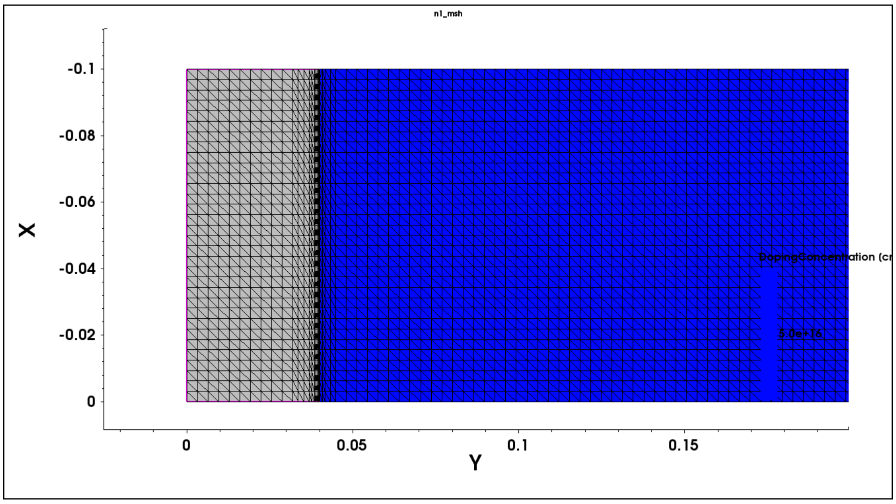

Figure 2: Schematic of the MS contact/Schottky Diode with meshing

4 Analysing the device

4.1 Band Diagram Analysis

$$\phi_s = \chi_1 + \frac{E_g}{2} - V_t ln \frac{n}{n_i} \tag{1}$$

Now

$\chi_1 = 4.05eV$,E$_g$ = 1.12eV and n = 5×10^{16}cm^{-3}.

$$E_g = 1.12\text{eV}$$

n = 5×10^{16}cm^{-3}.

From this we can calculate $\phi_s = 4.22$eV

4.1.1 Equilibrium

In equilibrium, we can observe that the Fermi levels are constant and there is no splitting of the Fermi levels.

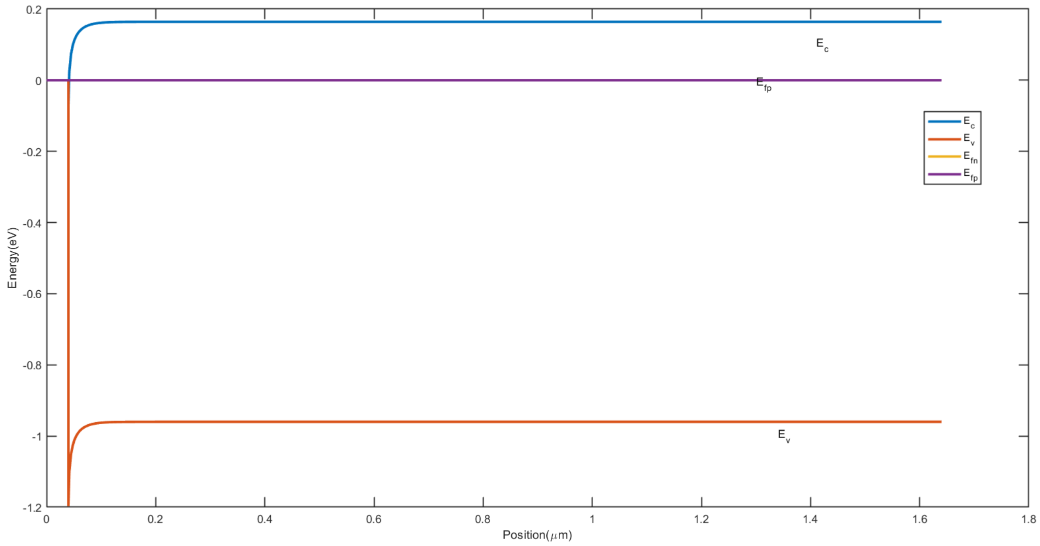

Figure 3: Energy band diagram $\phi_s(4.22eV) > \phi_m(4eV)$

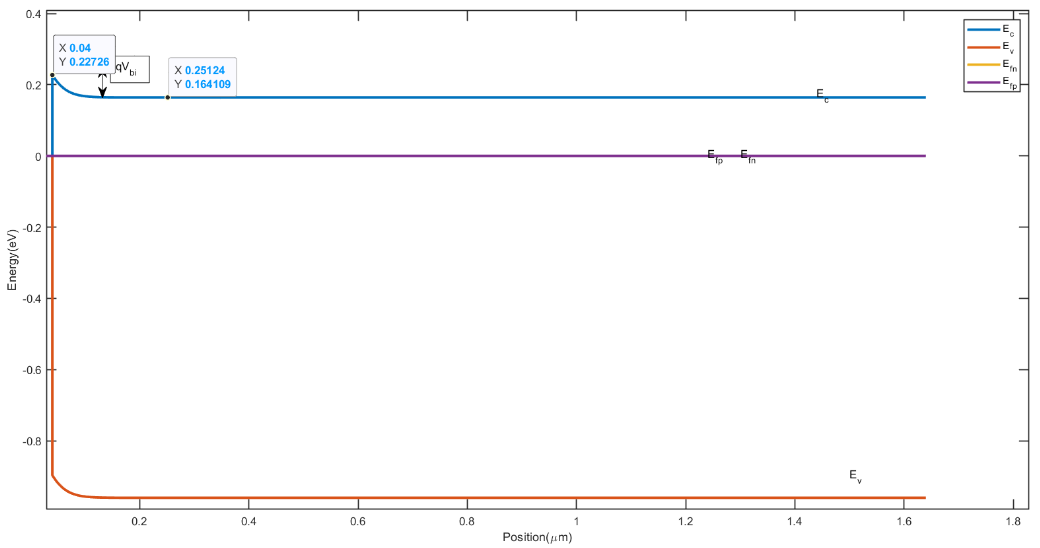

Figure 4: Energy band diagram $\phi_s(4.22eV) < \phi_m(4.3eV)$

When ϕ_s is greater than that of the ϕ_m we say it is an ohmic contact and the MS contact behaves as a resistor.
Considering a second case where metal work function is greater than that of semiconductor work function we say it works as a diode and the bending of the bands explains whether the MS is working as a diode or as a resistor.

4.1.2 Forward Bias for MS diode

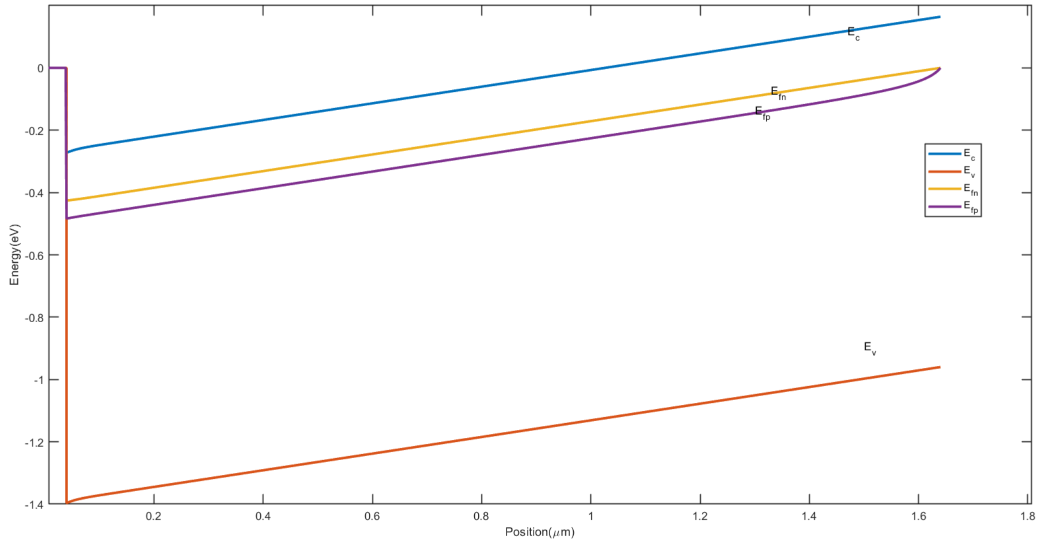

Figure 5: Energy band diagram in the Forward bias

4.1.3 Reverse Bias For MS diode

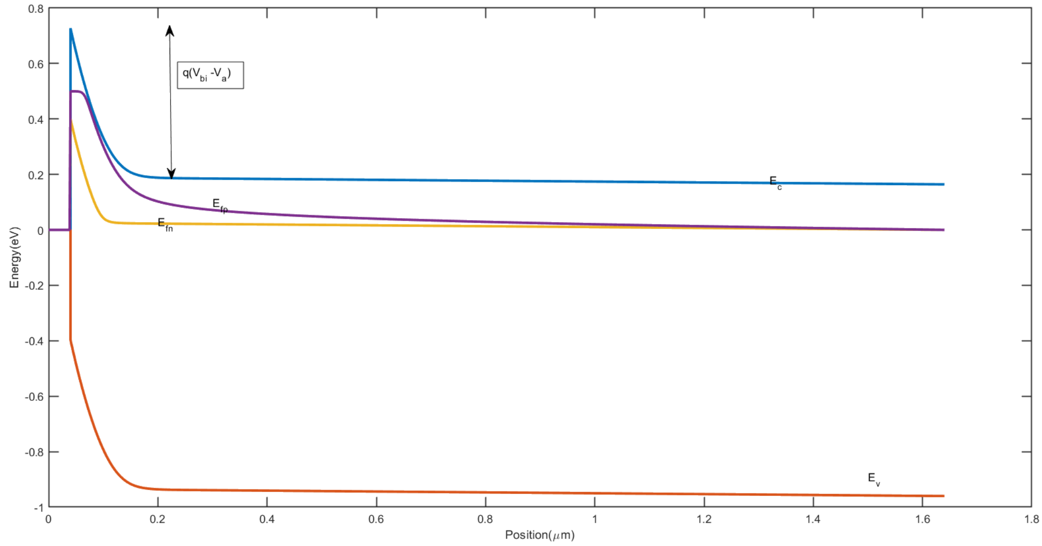

Figure 6: Energy Band diagram in the Reverse Bias

4.2 Show the built-in potential in each band diagram. Also, calculate the theoretical value

4.3 Calculating the Built in potential

The built in potential can be calculated using the similar idea as we have analysed the pn junction diode.

$$\phi_s = \chi_1 + \frac{E_g}{2} - V_t ln\frac{n}{n_i} \tag{2}$$

Now $\chi_1 = 4.05eV$,E_g = 1.12eV and n = 5×10^{16}cm$^{-3} Fromthiswecancalculate\phi_s$ = 4.22eV Now Built in potential can be calculated as

$$V_{bi} = \frac{1}{q}[\phi_m - \chi_1 - (E_c - E_f)] \tag{3}$$

$$(E_c - E_f) = \frac{E_g}{2} - V_t ln\frac{n}{n_i} \tag{4}$$

From this we get $V_{bi} = 0.079V$

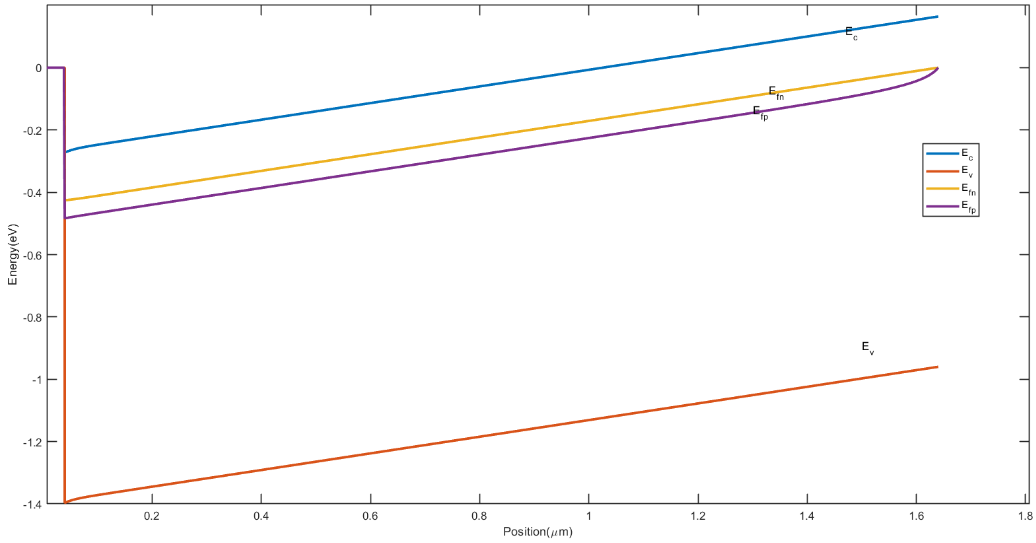

Figure 7: Energy band diagram Forward Bias

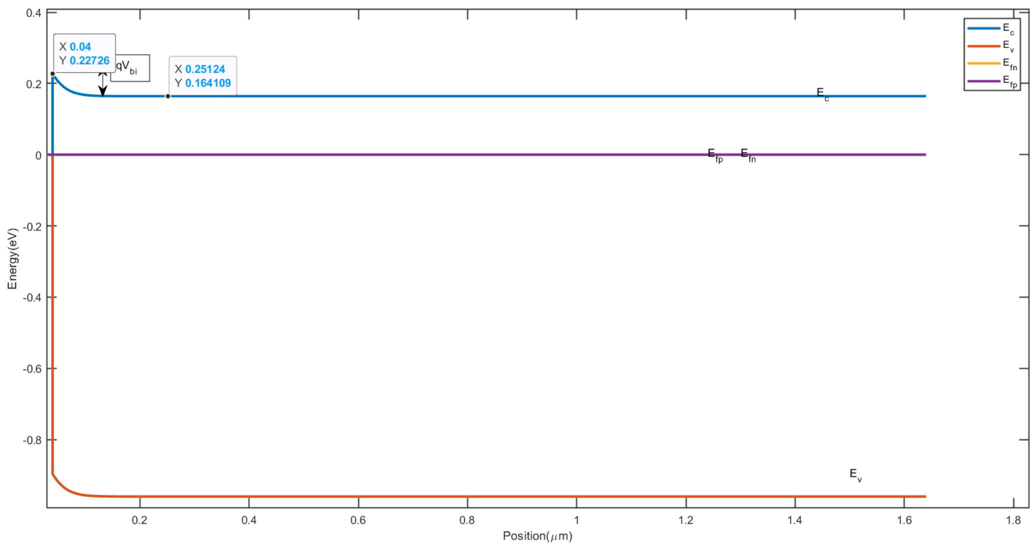

Figure 8: Energy band diagram in Equilibrium

From the above diagram we can calculate $V_{bi} = 0.22726 - .16400 = 0.06326V$

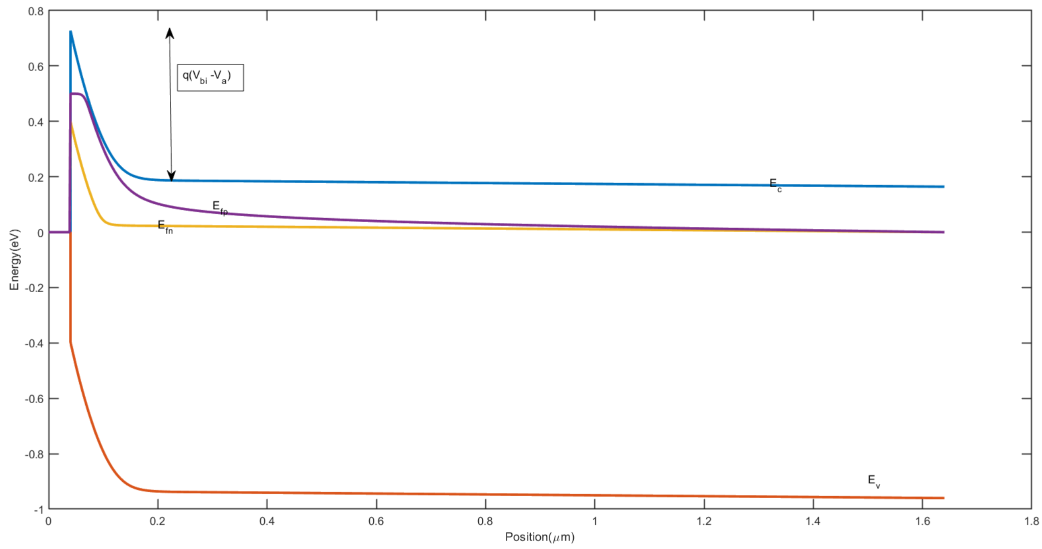

Figure 9: Energy band in Reverse bias

In the reverse bias also we can say that the total voltage across the junction from the diagram is $V_{bi} - (-V_a) = 0.559$V. Here we can say $V_{bi} = 0.059$V From the calculation we can say that $V_{bi} = 0.079V$ and $V_a = 0.5V$ The voltage across the junction is $V_{bi} + V_a = 0.579$V

4.4 Plot charge density, electric field, and electrostatic potential under equilibrium. Also, calculate the theoretical value

4.4.1 Electric Field Electrostatic potential and charge density for MS diode

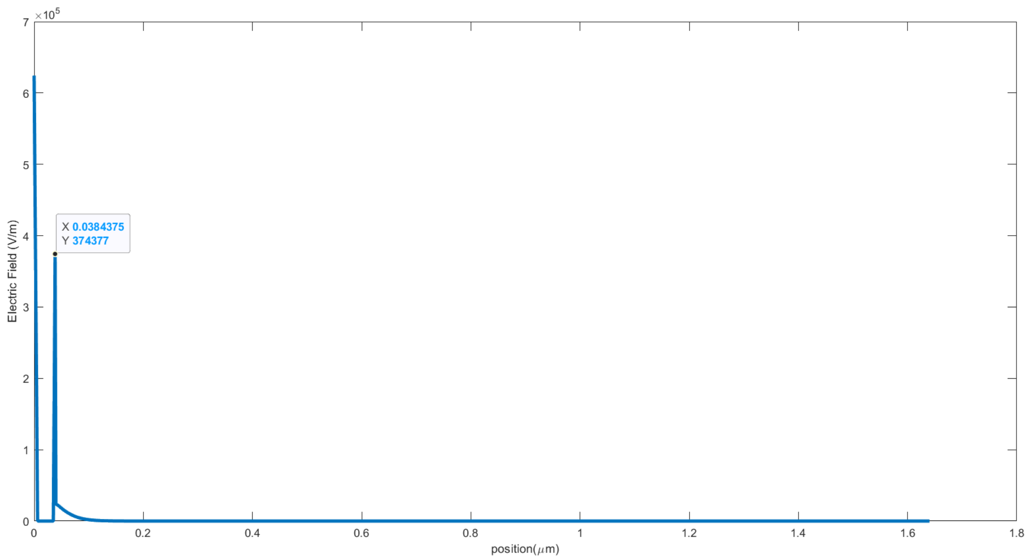

Figure 10: Electric field for MS diode $\phi_s < \phi_m$

Electric Field is given by

$$E(x) = \frac{-qN_d}{K_s\epsilon_o}(W - x)......0 \leq x \leq W \tag{5}$$

The peak value of electric field is given by

$$E_{max} = \frac{-qN_d}{K_s\epsilon_o}(W) \tag{6}$$

$$E_{max} = 3.0642 \times 10^5 V/m$$

The observed value is $3.6{\times}10^5$V/m

The electrostatic potential is given by integrating the electric field over distance.

$$V(x) = \frac{-qN_d}{2K_s\epsilon_o}(W-x)^2 \tag{7}$$

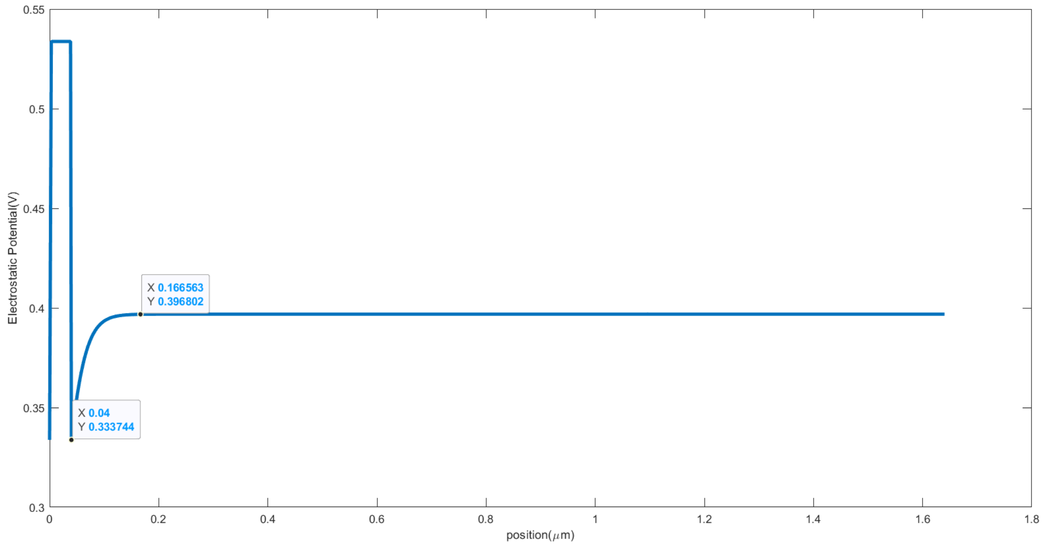

Figure 11: Electrostatic Potential $\phi_s < \phi_m$

V_{bi} = 0.06V i.e. the difference between the peak and the constant values. The calculated value by putting x=0 gives the value of V_{bi} as 0.079V.

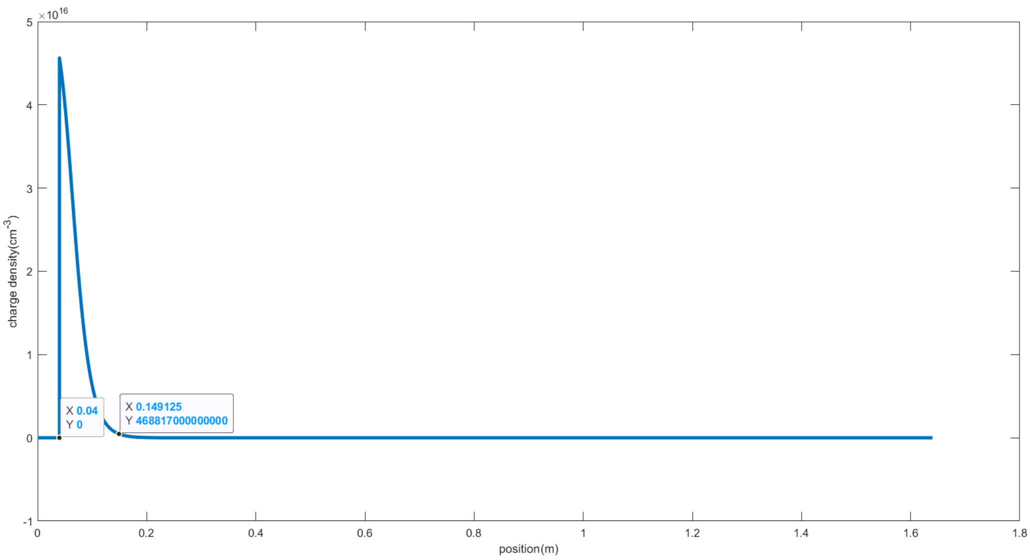

Figure 12: Charge density $\phi_s < \phi_m$

The W can be calculated as

$$W = [\frac{2K_s\epsilon_o V_{bi}}{qNd}]^{1/2} \tag{8}$$

$$W = 0.04\mu m$$

But the actual value comes around to be $0.10\mu m$ Charge density can be calculated as qN_d where N_d is given by 5×10^{16}. The charge density given in the plot shows the no. of charges rather than the total charge. So ideally it should be $5\times10^{16}cm^{-3}$ but from the plot it comes around to be $4.5\times10^{16}cm^{-3}$.

4.5 I-V characteristics of an MS Diode

The current in the MS diode is given by

$$I = I_s(e^{qVa/kT} - 1) \tag{9}$$

where I_s is given by

$$I_s = A(\frac{4\pi q m_o k^2}{h^3})T^2 e^{\frac{-\phi_B}{kT}} \tag{10}$$

$$\phi_B = \phi_m - \chi \tag{11}$$

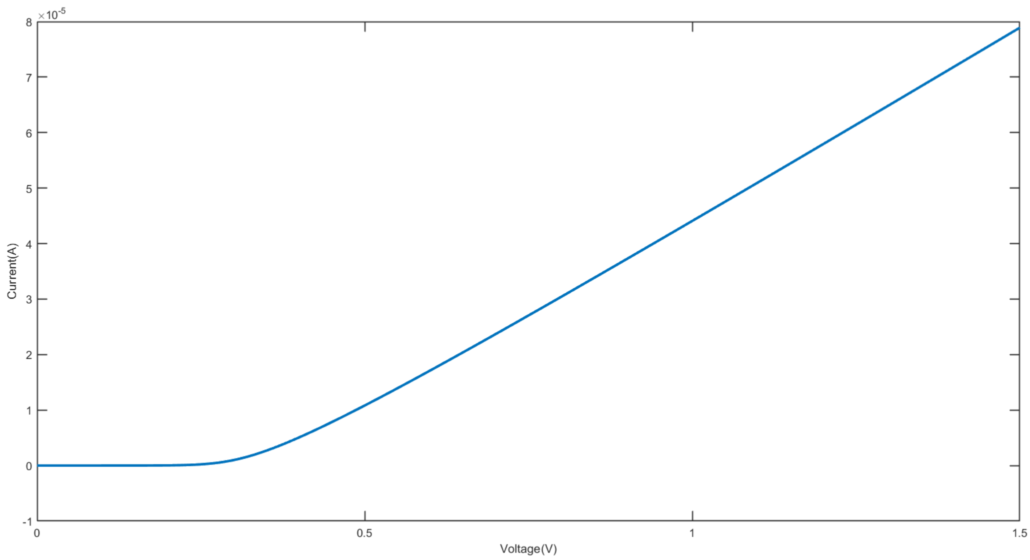

Figure 13: IV characteristics of an MS diode in forward bias

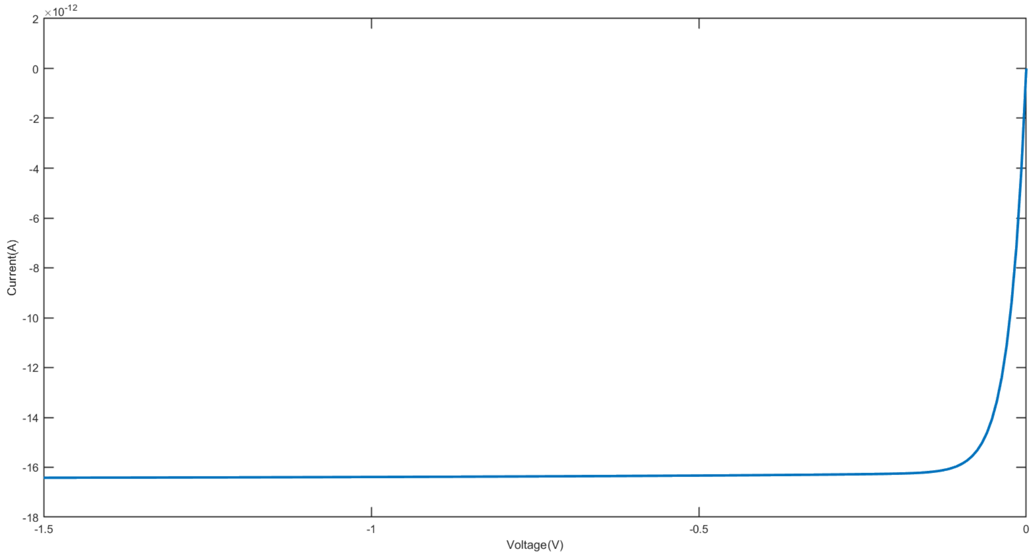

Figure 14: IV characteristics of an MS diode in reverse bias

4.6 CV characteristics for an MS Diode

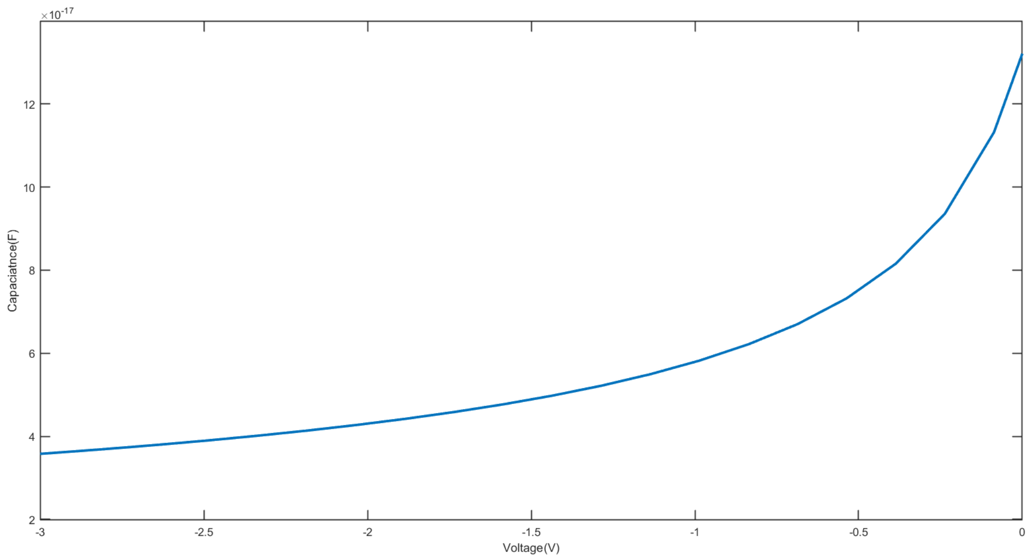

Figure 15: CV characteristics of an MS diode

The C-V is given by

$$C = \frac{K_s \epsilon_o A}{\sqrt{\frac{2K_s\epsilon_o(V_{bi}-V_a)}{qN_D}}} \tag{12}$$

The above equation implies that capacitance decreases as the reverse voltage is increased.

4.6.1 $\frac{1}{C^2}$ vs V characteristics of an MS diode

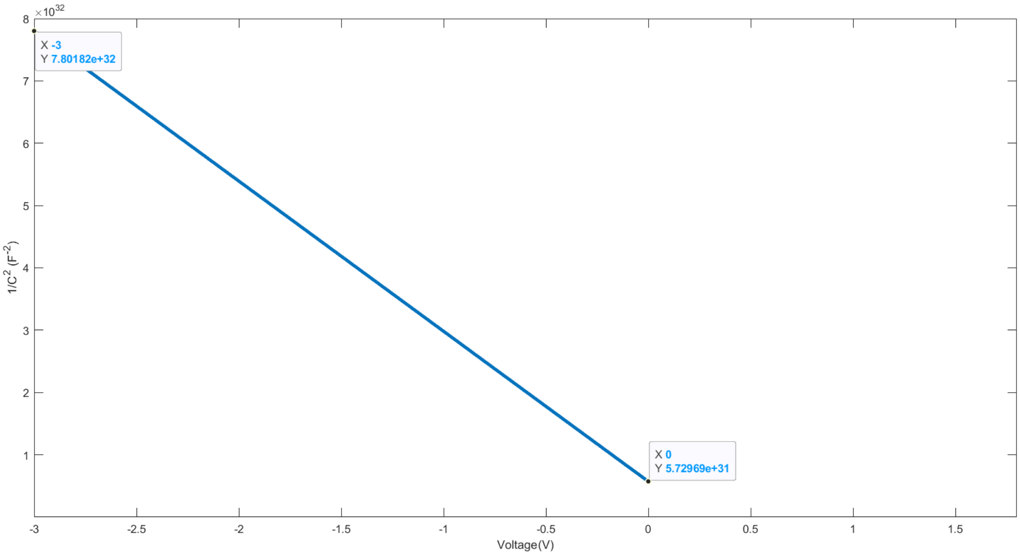

Figure 16: CV characteristics of an MS diode

Here we have plotted a characteristics for a work function of 4.5eV, hence we need to calculate the V_{bi} for this case and observe the result.

$$\phi_s = \chi_1 + \frac{E_g}{2} - V_t ln \frac{n}{n_i} \tag{13}$$

Now $\chi_1 = 4.05eV$,$E_g = 1.12$eV and n = 5×10^{16} From this we can calculate $\phi_s = 4.22$eV Now Built in potential can be calculated as

$$V_{bi} = \frac{1}{q}[\phi_m - \chi_1 - (E_c - E_f)] \tag{14}$$

$$(E_c - E_f) = \frac{E_g}{2} - V_t ln \frac{n}{n_i} \tag{15}$$

From this we get $V_{bi} = 0.28V$ From the plot we can say that the curve is a straight line with two points as (-3,7.8×10^{32}),(0, 5.7×10^{31}). From this we can calculate the equation of a straight line. Calculating the slope:

$$m = \frac{y_2 - y_1}{x_2 - x_1} \tag{16}$$

Slope comes to be -24.1×10^{31} From the equation of the line

$$y_2 - y_1 = m(x_2 - x_1) \tag{17}$$

The line comes out to be:

$$y - 5.7 \times 10^{31} = -24.1 \times 10^{31} x \tag{18}$$

Here the point where y cuts the x axis gives us the V_{bi} and the point is x= 0.236V. Now we can calculate the barrier height as qV_{bi} which is then equal to 0.236eV. Now if we have to calculate ϕ_B

$$qV_{bi} + (E_c - E_f) = \phi_B \tag{19}$$

$$0.236 + 0.56 - 0.389 = \phi_B$$

$$\phi_B = 0.407eV.$$

5 Conclusion

In this experiment we went through and analysed the MS contacts. First we provided a work function lesser than that of the semiconductor work function and plotted the band diagrams. This is the ohmic contact. Then we provided a work function greater than that of the semiconductor and analysed the band diagrams of the MS diode at different potentials. Then we plotted various other parameters like electric field, Electrostatic Potential and space charge at the equilibrium conditions. The IV characteristics and the CV characteristics of the MS diode were also plotted and analysed in the experiment. Lastly we plotted $\frac{1}{C^2}$ vs the applied volatge and calculated the barrier height.