



**Project 1**  
**Simulation of a PN Junction**

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## Introduction

This report examines the simulations of N<sup>+</sup>P junctions using the Sentaurus TCAD tool in our project. The project involves an N<sup>+</sup>P junction fabricated on a P-type silicon substrate with larger concentration of donor dopings. Our focus is to investigate the doping concentrations, built-in potential, and depletion width within a uniform doping profile. Then, we analyze the IV characteristic curves under reverse and forward bias and observe the effects of temperature on these biases. Lastly, we use a Gaussian doping profile, where we conduct a comparative analysis with the uniform profile with respect to the aforementioned parameters and characteristics.

## Methodology

Table 1 contains the symbols and definitions of the terms used throughout this report.

Table 1: Terminology

Symbol	Definition	Symbol	Definition
$k$	Boltzmann Constant ( $J/K$ )	$D_p, D_n$	Diffusion coefficient of the hole/electron ( $cm^2/s$ )
$T$	Temperature ( $K$ )	$E_g$	Band gap energy of the semiconductor (eV)
$\epsilon_s$	Electric Permittivity ( $F/cm$ ) (Silicon)	$n_i$	Electron or hole concentration in intrinsic semiconductor ( $cm^{-3}$ ) (Silicon)
$A$	Diode area ( $cm^2$ )	$L_p, L_n$	Hole and electron diffusion lengths (cm)
$V_R$	Reverse Bias Voltage (V)	$N_a, N_d$	Acceptor and donor concentrations ( $cm^{-3}$ )
$q$	Electron Charge ( $C$ )	$N_c, N_v$	Effective density of states in the conduction and valence band ( $cm^{-3}$ )

### A. Zero Bias, Uniform Doping Profiles

Certain parameters in the Sentaurus Device Editor (SDE) command file were changed, according to the values provided in the protocol (see Appendix A). The acceptor doping concentration  $N_a$  (The BoronActiveConcentration) was set to  $8 \times 10^{15} cm^{-3}$  and donor doping concentration  $N_d$  (PhosphorusActiveConcentration) was set to  $2 \times 10^{18} cm^{-3}$ . The total substrate thickness (tsub) was set to 10  $\mu m$ , total device width was set to 2  $\mu m$  and the junction depth was set to 1  $\mu m$ . Additionally, variable names electrode1 and electrode2, were changed to Cathode and Anode,

respectively. Lastly, in the SDevice command file, the temperature was set to 300K and the applied voltage was set to 0 by changing the “Value” within the Quasistationary function to 0 (see Appendix B).

The built-in potential is the electric potential difference across the depletion region during zero bias, where zero external voltage is applied. It's a result of the difference in the Fermi levels of the p-type and n-type materials. Hence, to calculate this potential we measure the difference between the highest and lowest values of the electrostatic potential. Whereas, the depletion region is where the charge carriers are depleted. Hence, to calculate the width of this region we can measure the width over which there is a change in the potential.

### **B. Reverse Bias, Uniform Doping Profiles**

To reverse bias a PN junction, a positive voltage is applied to the N region relative to the P region [1]. Therefore, in our simulation under the quasistationary function, we set the anode electrode (P-side) to have a negative voltage in the SDevice command file (see Appendix C). We experiment with large negative values, within the -60V to -90V range, to which the simulation *can* converge, in order to observe the reverse IV characteristic and the breakdown voltage. To calculate breakdown voltage, we pinpoint the largest reverse voltage (e.g. -75V) that can be applied without causing a sudden increase in the leakage current [2]. Then, we calculate the maximum electric field with the applied reverse bias voltage,  $V_R$ .

### **C. Forward Bias, Uniform Doping Profiles**

To forward bias a PN junction, the P region should have a higher potential. Therefore, in our simulation under the quasistationary section, we set the anode electrode (P-side) to have a positive voltage. To analyze the IV characteristic under forward bias between 0 to 1 V, we set the anode electrode to 1V in the SDevice command file (see Appendix D).

### **D. High Temperature, Uniform Doping Profiles**

To observe the effects of higher temperature on the IV characteristic, we set the junction temperature to 600°C (873.15 K) under the Physics function in the SDevice command files, and simulate a reverse bias of 10V (see Appendix E) and a forward bias of 1V (see Appendix F), in a methodology similar to Part B and C.

## E. Gaussian $n^+$ Doping Profiles

To examine the Gaussian doping profile, we use a Gaussian doping for the  $N^+$  region and a constant profile for the P region by modifying the SDE command file (see Appendix G). We repeat the processes in Parts A, B and C to calculate and compare values and characteristics with the uniform doping.

## Results and Discussion

### 1. Zero Bias, Uniform Doping Profiles

Using uniform doping profiles, with  $N_a = 8 \times 10^{15} \text{ cm}^{-3}$ ,  $N_d = 2 \times 10^{18} \text{ cm}^{-3}$  and junction depth of  $x_j = 1 \mu\text{m}$ , we verify the 1D and 2D impurity concentrations in *Figures 1 and 2*.

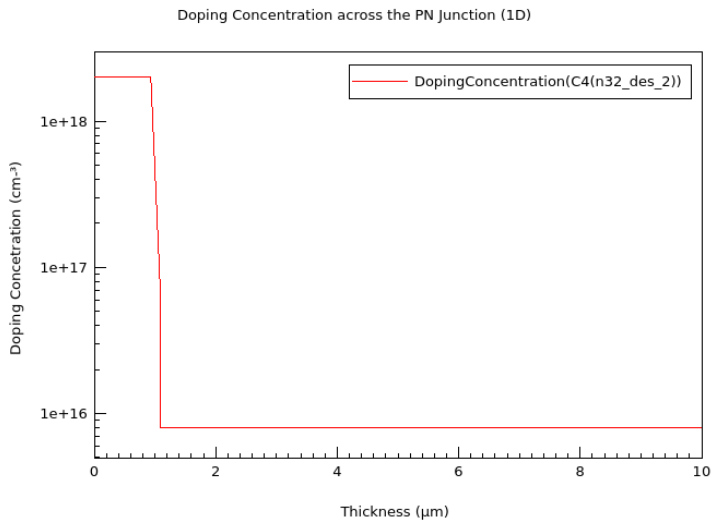


Figure 1: Doping Impurity Concentration in 1D

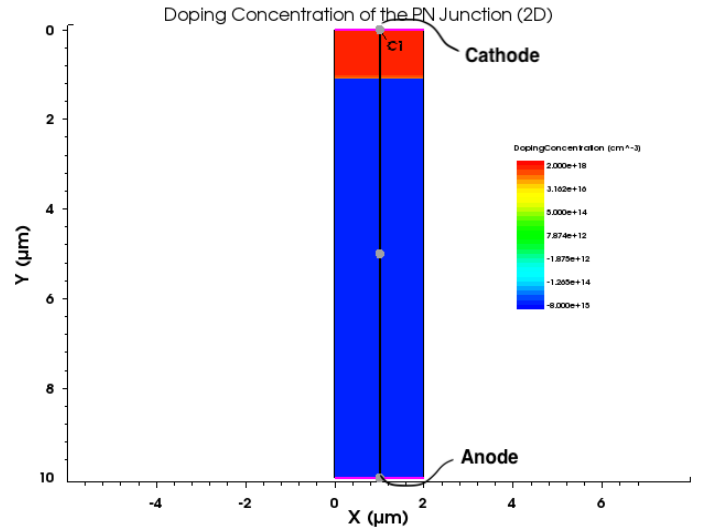


Figure 2: Doping Impurity Concentration in 2D

In *Figure 3*, the 1D plot illustrates the electrostatic potential across the junction and the depletion region width. The experimental built-in potential at 300 K is the difference between the max and min values of the electrostatic potential in *Figure 3*:  $0.47\text{V} - (-0.34)\text{V} = 0.81 \text{ V}$ .

The theoretical built-in potential at 300 K is

$$\Phi_{bi} = \frac{kT}{q} \ln\left(\frac{N_d \times N_a}{n_i^2}\right) = \frac{(1.381 \times 10^{-23} \text{ J/K})(300 \text{ K})}{1.6 \times 10^{-19} \text{ C}} \ln\left(\frac{2 \times 10^{18} \text{ cm}^{-3} \times 8 \times 10^{15} \text{ cm}^{-3}}{(1.5 \times 10^{10} \text{ cm}^{-3})^2}\right) = 0.826 \text{ V}$$

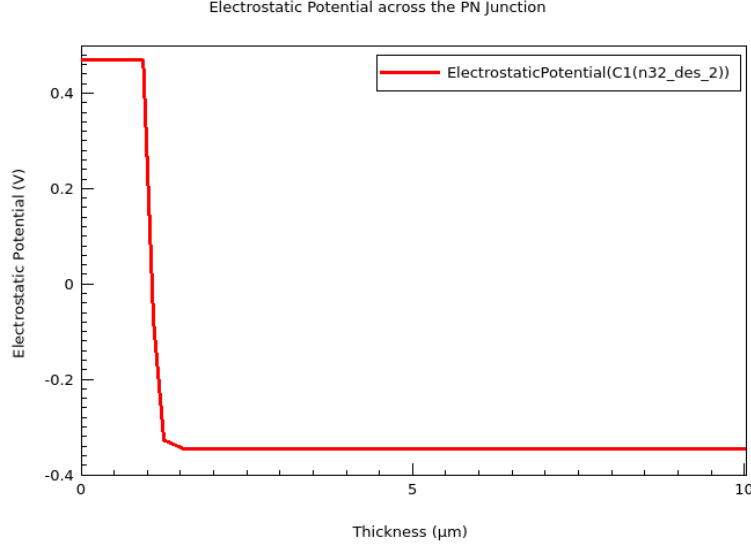


Figure 3: Electrostatic potential across the PN junction.

The experimental depletion region width is the region over which there is a change in potential in

Figure 3:  $1.27\mu\text{m} - 0.9\mu\text{m} = 0.37\mu\text{m}$ .

The theoretical depletion region width is

$$W = \sqrt{\frac{2\epsilon_s \Phi_{bi}}{q} \left( \frac{1}{N_d} + \frac{1}{N_a} \right)}$$

$$= \sqrt{\frac{2 (8.854 \times 10^{-14} \text{ F/cm} \times 11.7)(0.826 \text{ V})}{1.6 \times 10^{-19} \text{ C}} \left( \frac{1}{2 \times 10^{18} \text{ cm}^{-3}} + \frac{1}{8 \times 10^{15} \text{ cm}^{-3}} \right)} = 0.366 \mu\text{m}$$

Our experimental values for the built-in potential and depletion region width closely match with our theoretical values.

## 2. Reverse Bias, Uniform Doping Profiles

In Figure 4, the reverse IV characteristic when reverse bias voltage  $V_R$  of -75 V is applied is illustrated and the experimental breakdown voltage is seen at -63.64 V. This value matches the theoretical breakdown voltage at  $N_B = N_a = 8 \times 10^{15} \text{ cm}^{-3}$  (our lightly doped bulk concentration in the one-sided  $N^+P$  junction) which is -65 V, as noted in purple color in Figure 5.

The maximum electric field in the junction just before breakdown is:

$$\epsilon_{max} = \epsilon_{crit} = \sqrt{\frac{2qN_a(\Phi_{bi} + V_B)}{\epsilon_s}} = \sqrt{\frac{2 (1.6 \times 10^{-19} \text{ C})(8 \times 10^{15} \text{ cm}^{-3})(0.826 \text{ V} + 65 \text{ V})}{8.854 \times 10^{-14} \text{ F/cm} \times 11.7}} = 4.03326 \times 10^5 \text{ V/cm}$$

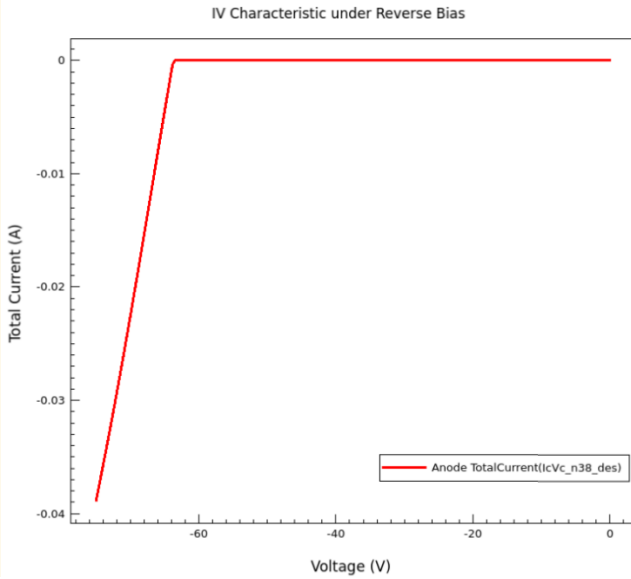


Figure 4: IV Characteristic under Reverse Bias

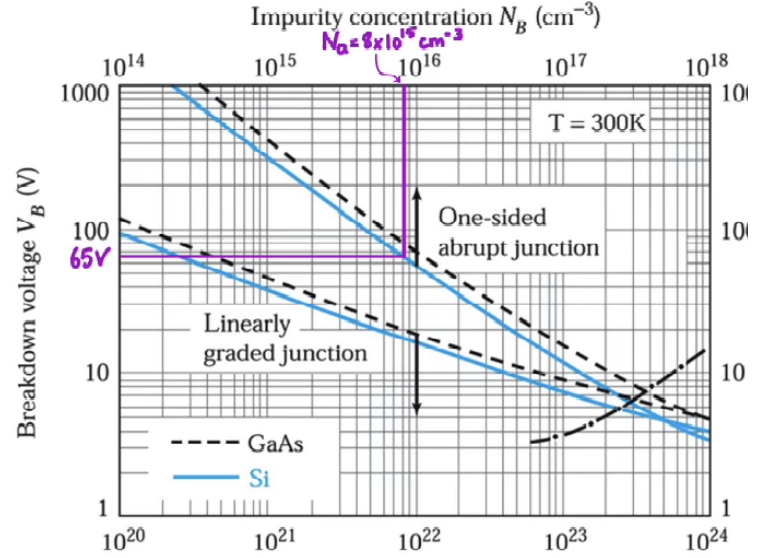


Figure 5: Concentration vs. Breakdown Voltage [3]

### 3. Forward Bias, Uniform Doping Profiles

In Figure 6, the forward bias IV characteristic is illustrated, and it is evident that the total current remains near zero until the applied forward bias voltage reaches a threshold value of 0.7 V. The forward bias of voltage reduces the barrier height [1]. Therefore, after this threshold value is surpassed, there's a direct exponential relationship between the voltage applied and the current. The more forward bias voltage, the smaller the barrier, and thus easier for the majority carriers to diffuse across the junction.

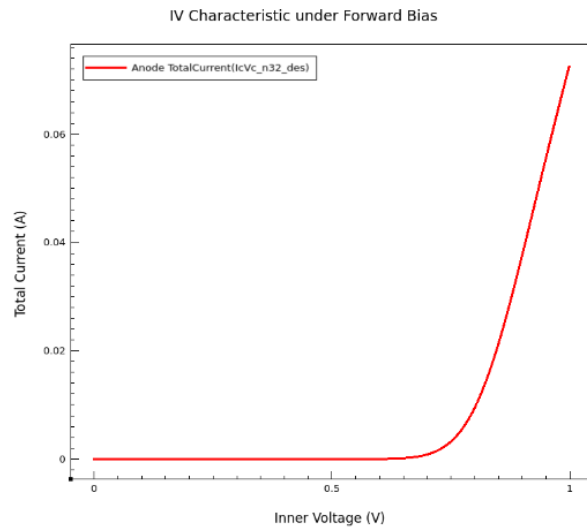


Figure 6: IV characteristic under forward bias when 1V applied at anode (at 300 K)

#### 4. High Temperature, Uniform Doping Profiles

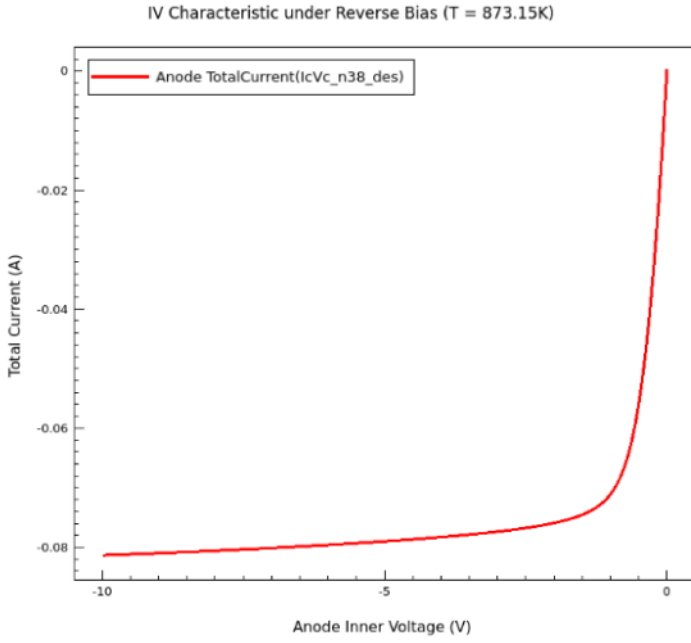


Figure 7: IV characteristics under reverse bias (-10V applied at anode) at 600°C

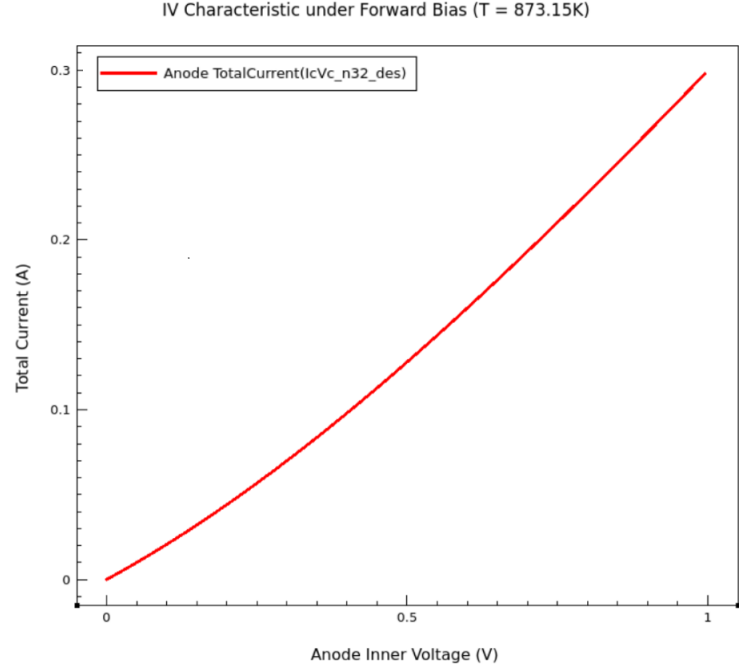


Figure 8: IV characteristics under forward bias (1V applied at anode) at 600°C

At higher temperatures intrinsic carrier concentration  $n_i$  increases by  $n_i = \sqrt{N_c N_v} \exp(\frac{-E_g}{2kT})$ .

The current in the diode is given by  $I = I_0(e^{qV/kT} - 1)$  where the reverse saturation current is

$$I_0 = Aq n_i^2 \left( \frac{D_p}{L_p N_d} + \frac{D_n}{L_n N_a} \right) [1].$$

The definitions of the terms in this equation are provided in Table

1 under the Methodology section. Therefore it takes a smaller voltage  $V$  for the diode to conduct a given current  $I$ , due to larger  $n_i$  at higher temperatures [2]. By comparing *Figure 6 and 8*, we can observe that, at increased temperatures, the slope of the IV curve is larger and the turn-on voltage is lower. In *Figure 7*, under reverse bias conditions, we observe a higher leakage current due to higher temperatures.

## 5. Gaussian $n^+$ Doping Profiles

1D and 2D doping concentrations of the junction are verified in the *Figures 9, 10 and 11*:

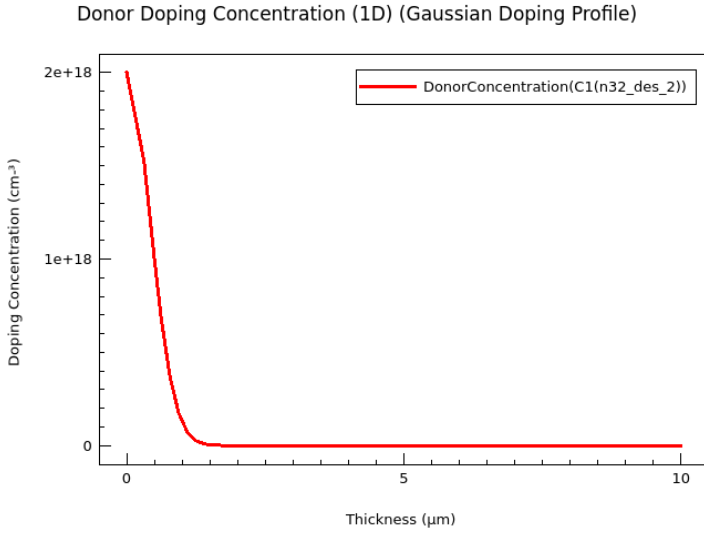


Figure 9: 1D donor doping concentration of the junction with Gaussian doping profile

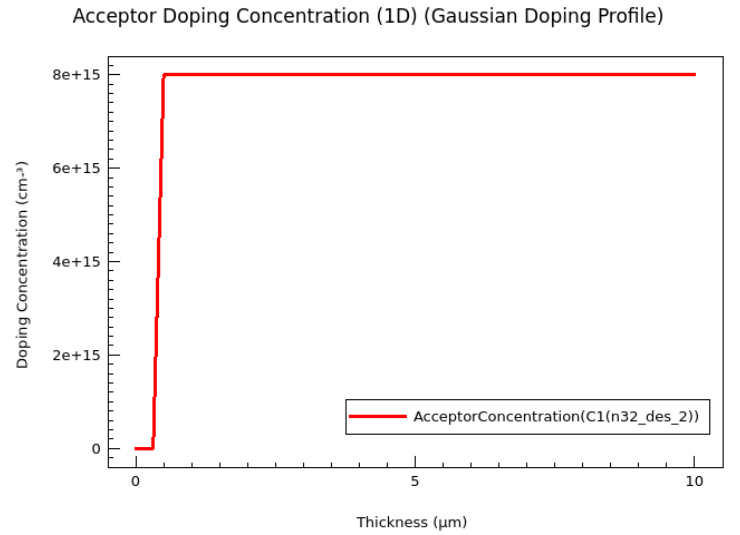


Figure 10: 1D acceptor doping concentration of the junction with Gaussian doping profile

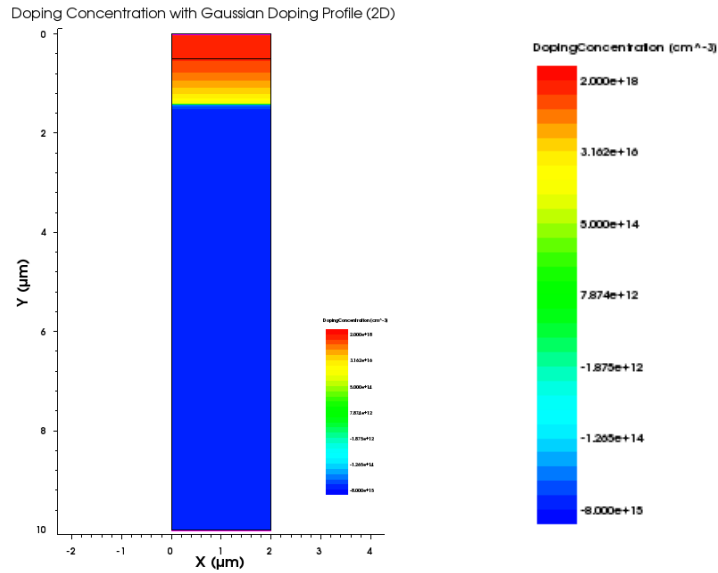


Figure 11: 2D doping concentration with Gaussian doping profile  
Doping concentration is  $2 \times 10^{18} \text{ cm}^{-3}$  in n-region to  $8 \times 10^{15} \text{ cm}^{-3}$  in p-region



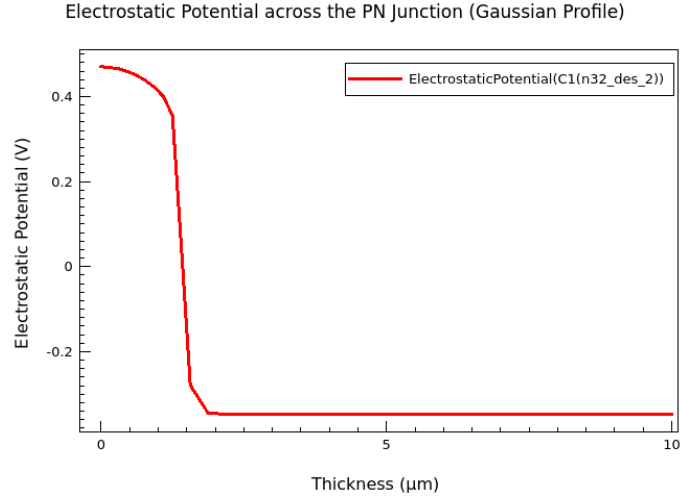


Figure 12: Electrostatic potential across PN junction under Gaussian doping profile ( $T=300K$ )

From Figure 12, the experimental built-in potential is the difference between the maximum and minimum values of the electrostatic potential:  $\Phi_{bi} = 3.46 \text{ V} - (-4.68 \text{ V}) = 0.814 \text{ V}$

The theoretical built-in potential is:

$$\Phi_{bi} = \frac{KT}{q} \ln\left(\frac{N_d \times N_a}{n_i^2}\right) = \frac{(1.381 \times 10^{-23} \text{ J/K})(300 \text{ K})}{1.6 \times 10^{-19} \text{ C}} \ln\left(\frac{2 \times 10^{18} \text{ cm}^{-3} \times 8 \times 10^{15} \text{ cm}^{-3}}{(1.08 \times 10^{10} \text{ cm}^{-3})^2}\right) = 0.843 \text{ V}$$

The experimental built-in potential is roughly the same as the theoretical one. In comparison with the uniform doping profile where the built-in potential was  $\Phi_{bi} = 0.826 \text{ V}$ , there is no significant difference.

From Figure 12, the experimental depletion region width is the region over which there is a change in potential:  $1.8 \mu\text{m} - 0 \mu\text{m} = 1.8 \mu\text{m}$ . The depletion region is significantly larger with the Gaussian doping profile, in comparison to the uniform doping profile where  $w_{\text{dep}}$  was  $0.37 \mu\text{m}$ .

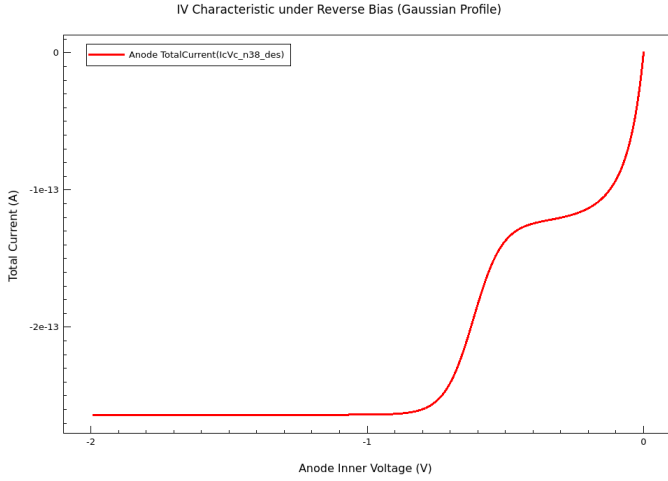


Figure 13: IV characteristic under reverse bias of  $-10V$  with Gaussian doping profile ( $T=300K$ )

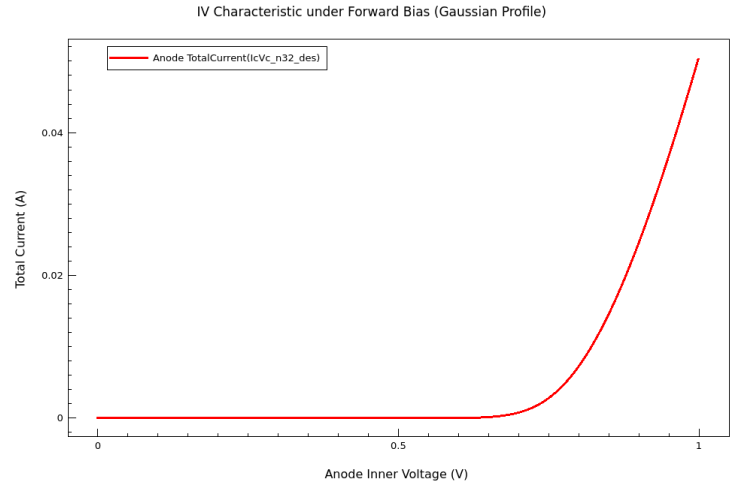


Figure 14: IV characteristic under forward bias of  $1V$  with Gaussian doping profile ( $T=300K$ )

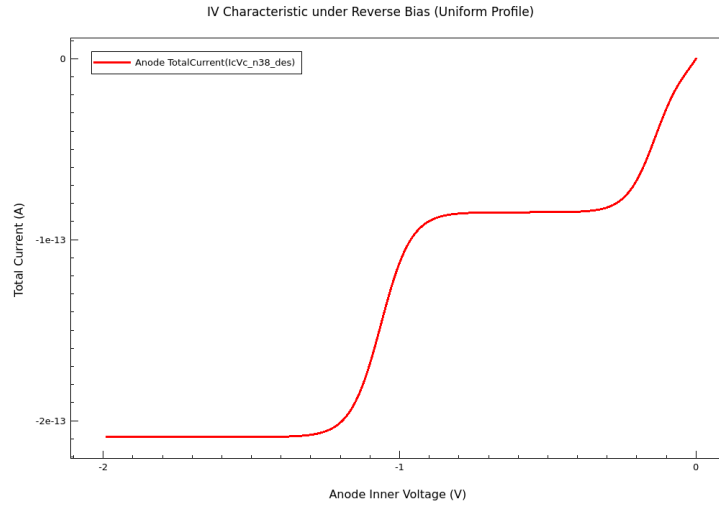
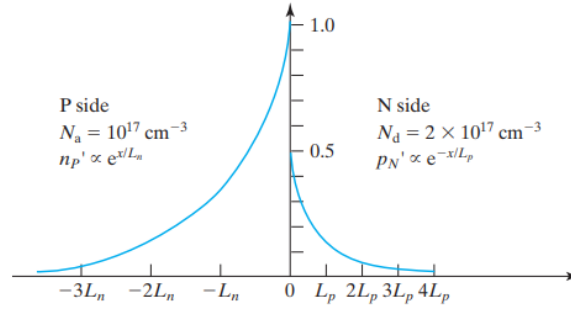


Figure 15: IV characteristic under reverse bias of  $-10V$  with uniform doping profile ( $T=300K$ )

Comparing Figure 13 and 15, the trends in the both reverse bias profiles are similar. However, in the junction with the Gaussian profile the curve starts to flatten out at a higher voltage of  $-0.8 V$  whereas this value is around  $-1.2 V$  in the uniformly doped diode. Comparing the IV characteristics under forward bias Figure 14 to Figure 6 from Part 3, we observe a similar pattern however the slope of the IV curve is slightly larger in the uniform doping profile.

To determine the diffusion lengths  $L_n$  and  $L_p$ , we start by calculating the excess concentrations of electrons ( $n'$ ) and holes ( $p'$ ). These concentrations are represented by  $p = p_o + p'$  and  $n = n_o + n'$ . By comparing the doping concentrations in two different states – one at equilibrium ( $n_o$  and  $p_o$ ) and the other under forward bias – we can identify the excess carrier concentrations. Then, normalizing  $n'$  and  $p'$  and creating a graph, similar to *Figure 16*, enables us to visually ascertain the diffusion lengths  $L_p$  and  $L_n$ .



*Figure 16: Example normalized excess electron and hole concentrations vs diffusion lengths*

## Conclusions

Our simulation of the N<sup>+</sup>P junction was executed under zero bias, reverse, and forward biases, and at two distinct temperature settings. The experimental findings for the zero bias condition indicated that the built-in potential and depletion width were in close approximation to their theoretical counterparts. Additionally, the experiment was extended to include a Gaussian doping profile, the results of which were benchmarked against those obtained from a uniform doping profile to conduct a comparison.

## References

1. C. Hu, “Chapter 4 PN and Metal-Semiconductor Junctions” in *Modern Semiconductor devices for integrated circuits*, Upper Saddle River (New Jersey): Prentice Hall, 2010.
2. “Breakdown voltage,” Wikipedia,  
[https://en.wikipedia.org/wiki/Breakdown\\_voltage#:~:text=Diodes%20and%20other%20semiconductors,-Diode%20I%2DV%20diagram&text=Breakdown%20voltage%20is%20a%20parameter,leakage%20current%20in%20the%20diode](https://en.wikipedia.org/wiki/Breakdown_voltage#:~:text=Diodes%20and%20other%20semiconductors,-Diode%20I%2DV%20diagram&text=Breakdown%20voltage%20is%20a%20parameter,leakage%20current%20in%20the%20diode). (Accessed Nov. 16, 2023).
3. S. M. Sze and M. K. Lee, *Semiconductor Devices: Physics and Technology*. Hoboken, NJ: Wiley, 2013.

## Appendix A

### Changes in the SDE command file (sde\_dvs.cmd) for Part A

```
; > Dimensions <
; Total thickness of the substrate set to 10 µm
(define tSub 10)

; > n type cSi layer <
; Total device width set to 2 µm
(sdegeo:create-rectangle (position 0 0 0) (position 2 tSub 0) "Silicon" "Subs" )

; > Electrode 1 <
; Electrode 1 defined as Cathode
(sdegeo:define-2d-contact (find-edge-id (position 0.2 0 0) ) "Cathode")

; > Electrode 2 <
; Electrode 2 defined as Anode
(sdegeo:define-2d-contact (find-edge-id (position 0.2 tSub 0) ) "Anode")

; > p region constant doping <
;  $N_a = 8 \times 10^{15} \text{ cm}^{-3}$ 
(sdedr:define-constant-profile "Const.Subs" "BoronActiveConcentration" 8e15)

; > n+ region <
;  $N_d = 2 \times 10^{18} \text{ cm}^{-3}$ 
(sdedr:define-constant-profile "doping.profile.nplusSi" "PhosphorusActiveConcentration" 2e18)
; Junction depth set to 1 µm
(sdedr:define-refeval-window "window.nplusSi" "Rectangle" (position 0 0 0.0) (position 2 1
0.0))
```

## Appendix B

### Changes in the Forward Bias SDevice command file (sdevice\_des.cmd) for Part A

; Temperature set to 300 K

Physics {

Temperature = 300

...

}

; Applied voltage set to 0

Quasistationary (

InitialStep=1e-9 Increment=1.5

MinStep=@<1e-8/1e10>@ MaxStep=1e-5

Goal { Name=Cathode Value=0 }

) { Coupled { Poisson Electron Hole }

## Appendix C

### Changes in the Reverse Bias SDevice command file (sdevice1\_des.cmd) for Part B

; Applied voltage set to -75

Quasistationary (

InitialStep=1e-9 Increment=1.5

MinStep=@<1e-8/1e10>@ MaxStep=1e-5

Goal { Name=Anode Value=-75 }

) { Coupled { Poisson Electron Hole }

## Appendix D

### Changes in the Forward Bias SDevice command file (sdevice\_des.cmd) for Part C

; Applied voltage set to 1

Quasistationary (

InitialStep=1e-9 Increment=1.5

MinStep=@<1e-8/1e10>@ MaxStep=1e-5

Goal { Name=Anode Value=1 }

) { Coupled { Poisson Electron Hole }

## Appendix E

### Changes in the Reverse Bias SDevice command file (sdevice1\_des.cmd) for Part D

; Temperature set to 873.15 K (600°C)

Physics {

Temperature=873.15

...

}

; Applied voltage set to -10

Quasistationary (

InitialStep=1e-9 Increment=1.5

MinStep=@<1e-8/1e10>@ MaxStep=1e-5

Goal { Name=Anode Value=-10 }

) { Coupled { Poisson Electron Hole }

## Appendix F

### Changes in the Forward Bias SDevice command file (sdevice\_des.cmd) for Part D

; Temperature set to 873.15 K (600°C)

Physics {

Temperature=873.15

...

}

; Applied voltage set to 1

Quasistationary (

InitialStep=1e-9 Increment=1.5

MinStep=@<1e-8/1e10>@ MaxStep=1e-5

Goal { Name=Anode Value=1 }

) { Coupled { Poisson Electron Hole }

## Appendix G

### Changes in the SDE command file (sde\_dvs.cmd) for Part E

```
; Structure definition
; Junction depth set to 0.5  $\mu\text{m}$ 
(sdegeo:create-rectangle
  (position 0.0 0.0 0.0) (position totalwidth 0.5 0.0) "Silicon" "nsub" )
(sdegeo:create-rectangle
  (position 0.0 0.5 0.0) (position totalwidth totalthickness 0.0) "Silicon" "psub" )

;Gaussian Doping
;Peak concentration (PeakVal) set to  $N_d=2 \times 10^{18} \text{ cm}^{-3}$ 
;Doping concentration at 0.5  $\mu\text{m}$  (ValueAtDepth) set to  $N_d=1 \times 10^{18} \text{ cm}^{-3}$ 
;Junction depth (Depth) set to 0.5  $\mu\text{m}$ 
;Gauss factor set to 0.8
(sdedr:define-gaussian-profile "nwell-doping-profile-gauss-hor"
  "PhosphorusActiveConcentration" "PeakPos" 0 "PeakVal" 2e18 "ValueAtDepth" 1e18
  "Depth" 0.5 "Gauss" "Factor" 0.8)
```