Diffusion 1D Simulator

Michelle King

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Contents

1 Given Constants

$$n_i = 1.5 \times 10^{10} cm^{-3}$$

2 Calculations

2.1 Built in Potential [2, p. 222]

Built in Potential [2, eq. 5.10]

$$V_{bi}[eV] = \frac{k_b T}{q} log(\frac{N_a N_d}{ni^2}) \tag{1}$$

Know: 1 eV = e J and J/C = V

$$\frac{k_b T}{q} = \frac{k_b T[\frac{eV}{K}][K]}{e[C]} \frac{e[J]}{[eV]} = \frac{k_b T[J]}{[C]} = k_b T \ [V] \tag{2}$$

For V_{bi} in Volts:

$$V_{bi}[V] = k_b T log(\frac{N_a N_d}{ni^2}) \tag{3}$$

2.2 Length of Device

Distance from 0 to n equilibrium [2, eq. 5.30a]

$$K_s \ \epsilon_0 = \epsilon$$

$$x_{n0} = \sqrt{\frac{2\epsilon}{q} \frac{N_A}{N_D(N_A + N_D)} V_{bi}}$$

Distance from 0 to p equilibrium [2, eq. 5.30b]

$$x_{p0} = \frac{N_D \ x_{n0}}{N_A}$$

Width of Depletion Region is the the total distance from equilibrium to equilibrium.

$$w_0 = x_{n0} + x_{p0}$$

Set the simulated device length proportional to the longest side

$$x_{max} = Scale \times Max(x_{n0}, x_{p0})$$

2.3 Mesh [4, p. 36]

Mesh size must be smaller than the Intrinsic Debye Length [4, eq. 3.12]

$$L_{di} = \sqrt{\frac{\epsilon k_b T}{n_i \ e^2}}$$

Unit Analysis:

$$L_{di} = \sqrt{\frac{\epsilon[\frac{F}{cm}] k_b T[eV]}{n_i[cm^{-3}] \ (e[C] * e)}}$$

$$L_{di} = \sqrt{\frac{\epsilon[F] k_b T[V]}{n_i[cm^{-2}] \ e[C]}}$$

$$F = \frac{C}{V}$$

$$L_{di} = \sqrt{\frac{\epsilon k_b T}{n_i \ e}[cm^2]}$$

$$L_{di} = \sqrt{\frac{\epsilon k_b T}{n_i \ e}}[cm]$$

Acceptor Extrinsic Debye Length

$$L_{da} = \sqrt{\frac{\epsilon k_b T}{N_a \ e^2}}$$

$$L_{da} = \sqrt{\frac{\epsilon k_b T}{N_a \ e}}[cm]$$

Donor Extrinsic Debye Length

$$L_{dd} = \sqrt{\frac{\epsilon k_b T}{N_d \ e^2}}$$

$$L_{dd} = \sqrt{\frac{\epsilon k_b T}{N_d \ e}} [cm]$$

Calculate dx as Minimum Extrinsic Debye Length

$$dx = Scale \ Factor \times Minimum(Lda, Ldd)$$

Scale Factor < 1 acts as a scale factor to further refine the mesh

Set the total number of array points in the mesh

$$n_{max} = int(\frac{x_{max}}{dx})$$

2.4 Doping Profile

From points 1 to nmax/2,

$$dop(i) = \frac{-N_a}{ni}$$

From points nmax/2 to nmax,

$$dop(i) = \frac{N_d}{ni}$$

2.5 Electric Field

$$E(x) = -\frac{d\psi}{dx}$$

$$E(i) = \frac{\psi_i - \psi_i + 1}{dx}$$

2.6 Carrier Density

$$density(i) = p(i) - n(i) - dop(i)$$

2.7 Conduction Band Energy

$$E_{CB}(i) = 0.5E_g - k_bT * psi(i)$$

3 Ohmic Contacts [1, p. 3-23]

"Ohmic contacts are implemented as simple Dirichlet boundary conditions where surface potential, electron concentration, and hole concentrations (ψ_s, n_s, p_s) are fixed. Minority and majority carier quasi-Fermi potentials are equal to the applied bias of the electrode, i.e. $\phi_n = \phi_p = V_{applied}$. The potential ψ_s is fixed at a value that is consistent with space charge neutrality, i.e."

$$n_s + N_A^- = p_s + N_D^+ \tag{4}$$

"Equation can be solved for ψ_s, n_s, p_s, since ϕ_n, ϕ_p, are known. If Boltzmann statistics are used, substitution of equations yields:"

$$n_s = \frac{1}{2}[(N_D^+ - N_A^-) + \sqrt{(N_D^+ - N_A^-)^2 + 4n_{ie}^2}] \tag{5}$$

$$p_s = \frac{n_{ie}^2}{n_s} \tag{6}$$

$$\psi_s = \phi_n + \frac{kT_L}{q}\ln(\frac{n_s}{n_{ie}}) = \phi_p - \frac{kT_L}{q}\ln(\frac{p}{n}) \tag{7}$$

4 Gummel Method [4, p. 40]

"Quasi-Linearization Procedure":

1. "Choose an initial guess for the potential" ψ

2. "Write the potential at the next iteration step as" $\psi_{new} = \psi + \delta\psi$ "and substitute into the linear Poisson Equation"

3. "Use the linearization" $exp(\pm\delta\psi) \approx 1 \pm \delta\psi$ "and discretize the resultant equation. This equation has a tridiagonal matrix form and is readily

solved for" $\delta\psi_i$

4. "Check for convergence. The residual... is calculated and convergence is achieved if the norm of the residual is smaller than a preset tolerance. If convergence is not achieved, return to step 2. In practice one might simply check the norm of the error"

$$\|\delta\psi\| \leq Tol$$

5 Poisson Solver

Linear Poisson Equation:

$$\frac{\partial^2\psi}{\partial x^2} = -\frac{e}{\epsilon_{sc}}[p - n + N_d(x) - N_a(x)] \tag{8}$$

where electron and hole density are defined as:

$$n = n_i exp(\psi) \tag{9}$$

$$p = n_i exp(-\psi) \tag{10}$$

This expands to:

$$\frac{\partial^2\psi}{\partial x^2} = -\frac{e}{\epsilon_{sc}}[n_i exp(\psi) + n_i exp(-\psi) + \frac{N_a(x) - N_d(x)}{n_i}] \tag{11}$$

Set $\psi \to \psi + \delta$

The second derivative on the left side remains unchanged:

$$\frac{\partial^2\psi}{\partial x^2} \to \frac{\partial^2(\psi + \delta\psi)}{\partial x^2} = \frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\delta\psi}{\partial x^2} = \frac{\partial^2\psi}{\partial x^2} \tag{12}$$

Substitute into the Linear Poisson Equation:

$$\frac{\partial^2\psi}{\partial x^2} = -\frac{e}{\epsilon_{sc}}[n_i exp(-\psi + \delta\psi) - n_i exp(\psi + \delta\psi) + N_a(x) - N_d(x)] \tag{13}$$

Expand the exponentials:

$$\frac{\partial^2\psi}{\partial x^2} = -\frac{e}{\epsilon_{sc}}[n_i exp(-\psi)exp(\delta\psi) - n_i exp(\psi)exp(\delta\psi) + N_a(x) - N_d(x)] \quad (14)$$

Assume: $exp(\delta\psi) = 1 + \delta\psi$

$$\frac{\partial^2\psi}{\partial x^2} = -\frac{e}{\epsilon_{sc}}[n_i exp(-\psi) - n_i exp(\psi) + N_a(x) - N_d(x)] + \delta\psi[n_i exp(-\psi) - n_i exp(\psi)] \quad (15)$$

Reduce to original terms:

$$\frac{\partial^2\psi}{\partial x^2} = -\frac{e}{\epsilon_{sc}}(p - n + C_i) + \frac{e}{\epsilon_{sc}}\delta(p + n) \quad (16)$$

Absorb factor of $\frac{e}{\epsilon_{sc}}$ to reduce computation time:

$$\frac{\partial^2\psi}{\partial x^2} = (p - n + C_i) + \delta(p + n) \quad (17)$$

Finite Difference Scheme:

$$f''(x_0) = \frac{f(x_0 + \delta x) - 2f(x_0) + f(x_0 - \delta x)}{\delta x^2} \quad (18)$$

Finite Difference in Terms of Mesh Points:

$$\frac{\partial^2\psi}{\partial x^2} = \frac{\psi_{i+1}^{n+1} - 2\psi_i^{n+1} + \psi_{i-1}^{n+1}}{\Delta^2} \quad (19)$$

Finite Difference Representation of Linear Poisson Equation:

$$\underbrace{\frac{1}{\Delta^2}}_{b_i}\psi_{i+1}^{n+1} - \underbrace{(\frac{2}{\Delta^2} + n_i + p_i)}_{a_i}\psi_i^{n+1} + \underbrace{\frac{1}{\Delta^2}}_{c_i}\psi_{i-1}^{n+1} = -(p_i - n_i + C_i) - (p_i + n_i)\psi_i^n \quad (20)$$

$$= -(exp(-\psi_i) - exp(\psi_i) + dop_i) - (exp(-\psi_i) + exp(\psi_i))\psi_i^n \tag{21}$$

$$= exp(\psi_i) - exp(-\psi_i) - dop_i - (exp(-\psi_i) + exp(\psi_i))\psi_i^n \tag{22}$$

6 LU Decomposition

6.1 Derivation

Begin with a matrix A and apply Ohmic boundary conditions:

$$A = \begin{bmatrix} a_1 & c_1 & \dots\dots\dots\dots & 0 \\ b_2 & a_2 & c_2 & \dots\dots\dots\dots \\ \dots\dots\dots\dots & \dots\dots\dots\dots & \dots\dots\dots\dots & \dots\dots\dots\dots \\ \dots\dots & b_{n-1} & a_{n-1} & c_{n-1} \\ 0 & \dots\dots\dots & b_n & a_n \end{bmatrix} = \underbrace{\begin{bmatrix} 1 & 0 & \dots\dots\dots\dots & 0 \\ b_2 & a_2 & c_2 & \dots\dots\dots\dots \\ \dots\dots\dots\dots & \dots\dots\dots\dots & \dots\dots\dots\dots & \dots\dots\dots\dots \\ \dots\dots & b_{n-1} & a_{n-1} & c_{n-1} \\ 0 & \dots\dots\dots & 0 & 1 \end{bmatrix}}_{\text{Ohmic BC Applied}}$$

A Matrix A can be separated into multiplied lower and upper triangular matrices

$$A = LU$$

$$\underbrace{\begin{bmatrix} a_1 & c_1 & \dots\dots\dots\dots & 0 \\ b_2 & a_2 & c_2 & \dots\dots\dots\dots \\ \dots\dots\dots\dots & \dots\dots\dots\dots & \dots\dots\dots\dots & \dots\dots\dots\dots \\ \dots\dots & b_{n-1} & a_{n-1} & c_{n-1} \\ 0 & \dots\dots\dots & b_n & a_n \end{bmatrix}}_{\text{Matrix A}} = \underbrace{\begin{bmatrix} 1 & \dots\dots\dots\dots & 0 \\ \beta_2 & 1 & \dots\dots\dots \\ \dots & \beta_3 \; 1 & \dots\dots \\ \dots\dots\dots\dots & \dots\dots\dots\dots & \dots\dots\dots\dots \\ 0 & \dots\dots \; \beta_n & 1 \end{bmatrix}}_{\text{Lower Triangular Matrix L}} \underbrace{\begin{bmatrix} \alpha_1 & c_1 & \dots\dots & 0 \\ \dots & \alpha_2 & c_2 & \dots\dots \\ \dots\dots\dots\dots & \dots\dots\dots\dots & \dots\dots\dots\dots & \dots\dots\dots\dots \\ \dots\dots\dots & & \alpha_{n-1} & c_{n-1} \\ 0 & \dots\dots\dots\dots & & \alpha_n \end{bmatrix}}_{\text{Upper Triangular Matrix U}}$$

$Ax = f$
$LUx = f$
$Ux = y$

$Ly = f$

Find L & U from A
$\alpha_1 = a_1$
$\beta_k = \frac{b_k}{\alpha_{k-1}}$
$\alpha_k = a_k - \beta_k c_{k-1}$

Forward & Back Substitution
$g_1 = f_1$
$g_i = f_i - \beta_i g_i$
$i = 2, 3, \ldots, n$

$x_n = \frac{g_n}{\alpha_n}$
$x_i = \frac{g_i - c_i x_{i+1}}{\alpha_i}$
$i = n-1, \ldots, 2, 1$

6.2 Relation to Physics

$$A = \begin{bmatrix} 1 & 0 & \ldots\ldots\ldots\ldots & & 0 \\ b_2 & a_2 & c_2 & & \ldots\ldots\ldots\ldots \\ \ldots\ldots\ldots\ldots & \ldots\ldots & \ldots\ldots & \ldots\ldots & \ldots\ldots \\ \ldots\ldots & & b_{n-1} & a_{n-1} & c_{n-1} \\ 0 & \ldots\ldots\ldots & & 0 & 1 \end{bmatrix}$$

$$x = \begin{bmatrix} \psi_1 \\ \psi_2 \\ \vdots \\ \psi_n \end{bmatrix}$$

$$f = \begin{bmatrix} exp(\psi_1) - exp(-\psi_1) - dop_1 - exp(\psi_1) * (exp(\psi_1) + exp(-\psi_1)) \\ exp(\psi_2) - exp(-\psi_2) - dop_2 - exp(\psi_2) * (exp(\psi_2) + exp(-\psi_2)) \\ \vdots \\ exp(\psi_n) - exp(-\psi_n) - dop_n - exp(\psi_n) * (exp(\psi_n) + exp(-\psi_n)) \end{bmatrix}$$

7 SRH Concentation Dependent Lifetime Model [1, p. 3-60]

Shockley-Read-Hall Recombination Model

7.1 Equation

$$R_{SRH} = \frac{pn - n_i^2}{\tau_p[n + n_i exp(\frac{ETRAP}{kT})] + \tau_n[p + n_i exp(\frac{-ETRAP}{kT})]} \tag{23}$$

Assume that the difference between the trap energy level and intrinsic Fermi level, $ETRAP = 0$, so that recombination can be simplified to:

$$R_{SRH} = \frac{pn - n_i^2}{\tau_p[n + n_i] + \tau_n[p + n_i]} \tag{24}$$

The definitions of electron and hole concentration are:

$$n = n_i exp(\psi_i^n) \tag{25}$$

$$p = n_i exp(-\psi_i^n) \tag{26}$$

For the calculations in our model, the factor for the intrinsic concentration is removed:

$$n(i) = exp(\psi_i^n) \tag{27}$$

$$p(i) = exp(-\psi_i^n) \tag{28}$$

Expands to:

$$R_{SRH} = \frac{(n_i exp(-\psi_i^n))(n_i exp(\psi_i^n)) - n_i^2}{\tau_p[(n_i exp(\psi_i^n)) + n_i] + \tau_n[(n_i exp(-\psi_i^n)) + n_i]} \tag{29}$$

$$R_{SRH} = \frac{n_i^2(exp(-\psi_i^n)exp(\psi_i^n) - 1)}{n_i(\tau_p[exp(\psi_i^n) + 1] + \tau_n[exp(-\psi_i^n) + 1])} \tag{30}$$

$$R_{SRH} = \frac{n_i(exp(-\psi_i^n)exp(\psi_i^n) - 1)}{\tau_p[exp(\psi_i^n) + 1] + \tau_n[exp(-\psi_i^n) + 1]} \quad (31)$$

$$R_{SRH} = \frac{n_i(p(i)n(i)) - 1)}{\tau_p[n(i) + 1] + \tau_n[p(i) + 1]} \quad (32)$$

$$\tau_n = \frac{TAUN0}{1 + N/(NSRHN)} \quad (33)$$

$$\tau_p = \frac{TAUP0}{1 + N/(NSRHP)} \quad (34)$$

Parameters (Table 3-36 in Atlas)		
Parameter	Value	Units
TAUN0	$1e-7$	s
NSRHN	$5e16$	cm^{-3}
TAUP0	$1e-7$	s
NSRHP	$5e16$	cm^{-3}

7.2 Units

$$\tau = \frac{TAU0\ [s]}{1 + N[cm^{-3}]/(NSRH[cm^{-3}])} \quad (35)$$

$$\tau = \frac{TAU0\ [s]}{1 + N/(NSRH)} \quad (36)$$

This leaves us with τ in seconds, which is what we expect

$$R_{SRH} = \frac{pn[cm^{-6}] - n_i^2[cm^{-6}]}{\tau_p[s][n + n_i][cm^{-3}] + \tau_n[s][p + n_i][cm^{-3}]} \quad (37)$$

$$R_{SRH} = \frac{pn[cm^{-3}] - n_i^2[cm^{-3}]}{\tau_p[s][n + n_i] + \tau_n[s][p + n_i]} \quad (38)$$

This leaves us with R_{SRH} in units of $[cm^{-3}/\text{sec}]$

Since this number is with respect to real space and not the mesh,

8 The Arora Model for Low Field Mobility [1, p. 3-35]

$$\mu_{n0} = \mu_{1n}(\frac{T_L}{300})^{\alpha_n} + \frac{\mu_{2n}(\frac{T_L}{300})^{\beta_n}}{1 + \frac{N}{N_{critn}(\frac{T_L}{300})^{\gamma_n}}}$$

$$\mu_{p0} = \mu_{1p}(\frac{T_L}{300})^{\alpha_p} + \frac{\mu_{2p}(\frac{T_L}{300})^{\beta_p}}{1 + \frac{N}{N_{critp}(\frac{T_L}{300})^{\gamma_p}}}$$

Parameters (Table 3-19 in Atlas)		
Parameter	Value	Units
MU1N	88	$cm^2/(Vs)$
MU1P	54.3	$cm^2/(Vs)$
MU2N	1252.0	$cm^2/(Vs)$
MU2P	407.0	$cm^2/(Vs)$
ALPHAN	-0.57	$unitless$
ALPHAP	-0.57	$unitless$
BETAN	-2.33	$unitless$
BETAP	-2.23	$unitless$
GAMMAN	2.546	$unitless$
GAMMAP	2.546	$unitless$
NCRITN	$1.43e17$	cm^{-3}
NCRITP	$2.67e17$	cm^{-3}

9 Field Dependent Mobility

Field Dependent Mobility Model

$$\mu(E) = \frac{\mu_0}{[1 + (\frac{\mu_0 E}{v_{sat}})^\beta]]^{1/\beta}}$$

where

$$\beta = \begin{cases} 1 & electrons \\ 2 & holes \end{cases}$$

Saturation Velocity [cm/s]

$$v_{sat}(T) = \frac{2.4 * 10^7}{1 + 0.8exp(\frac{T_L}{600})}$$

but $E(x) = -\frac{d\psi}{dx}$ so

$$\mu(E) = \frac{\mu_0}{[1 + (\frac{-\mu_0 \frac{d\psi}{dx}}{v_{sat}})^\beta]]^{1/\beta}}$$

We need to discretize this:

$$\mu(E) = \frac{\mu_0}{[1 + (\frac{-\mu_0 \frac{\psi_{i+1} - \psi_i}{\Delta}}{v_{sat}})^\beta]]^{1/\beta}}$$

10 Diffusion From Mobility [2]

Einstein Relation (Electrical mobility equation)

$$D = \frac{k_b T}{q} \mu$$

11 Sharfetter-Gummel Discretization Scheme [4, p.169]

11.1 Discretize Current

Current Equations

$$J_n = qn(x)\mu_n E(x) + qD_n \frac{dn}{dx} \tag{39}$$

$$J_p = qp(x)\mu_p E(x) - qD_p \frac{dp}{dx} \tag{40}$$

Continuity Equations

$$\frac{\partial n}{\partial t} = \frac{1}{q} \nabla \cdot \mathbf{J}_n + U_n \tag{41}$$

$$\frac{\partial p}{\partial t} = -\frac{1}{q}\nabla \cdot \mathbf{J}_p + U_p \tag{42}$$

Where U_n and U_p are the generation rates for electrons and holes respectively. Put electric field in terms of potential in current equations

$$J_n = qn(x)\mu_n(-\frac{d\psi}{dx}) + qD_n\frac{dn}{dx} \tag{43}$$

$$J_p = qp(x)\mu_p(-\frac{d\psi}{dx}) - qD_p\frac{dp}{dx} \tag{44}$$

Discretize the Current Equations

$$J_{i+\frac{1}{2}} = q\mu_n n_{i+\frac{1}{2}}(-\frac{\psi_{i+1}-\psi_i}{\Delta}) + qD_n\frac{n_{i+1}-n_i}{\Delta} \tag{45}$$

$$J_{i+\frac{1}{2}} = q\mu_p p_{i+\frac{1}{2}}(-\frac{\psi_{i+1}-\psi_i}{\Delta}) - qD_p\frac{p_{i+1}-p_i}{\Delta} \tag{46}$$

Approximate $n_{i+\frac{1}{2}}$ as an average of the two existing points around it.

$$n_{i+\frac{1}{2}} = \frac{n_{i+1}+n_i}{2} \tag{47}$$

$$p_{i+\frac{1}{2}} = \frac{p_{i+1}+p_i}{2} \tag{48}$$

Rewrite current equation

$$J_{i+\frac{1}{2}} = n_{i+1}[-\frac{1}{2}q\mu_n(\frac{\psi_{i+1}-\psi_i}{\Delta}) + q\frac{D_n}{\Delta}] - n_i[\frac{1}{2}q\mu_n(\frac{\psi_{i+1}-\psi_i}{\Delta}) + q\frac{D_n}{\Delta}] \tag{49}$$

$$J_{i+\frac{1}{2}} = -p_{i+1}[\frac{1}{2}q\mu_p(\frac{\psi_{i+1}-\psi_i}{\Delta}) + q\frac{D_p}{\Delta}] + p_i[-\frac{1}{2}q\mu_p(\frac{\psi_{i+1}-\psi_i}{\Delta}) + q\frac{D_p}{\Delta}] \tag{50}$$

11.2 Solved Discretized Current

The discretization of the continuity equation for electrons and holes is:

$$\frac{J_{i+\frac{1}{2}} - J_{i-\frac{1}{2}}}{\Delta} = q(R_i - G_i) \tag{51}$$

where R and G are Recombination and Generation Rates

Discretized J can be found by:

$$J_{i+\frac{1}{2}} = qD_{i+\frac{1}{2}} \frac{n_{i+1}B(\psi'_{i+1} - \psi'_i) - n_i B(\psi'_i - \psi'_{i+1})}{\Delta} \tag{52}$$

where

$$\psi' = \frac{q}{k_b T}\psi \tag{53}$$

And

$$J_{i-\frac{1}{2}} = qD_{i-\frac{1}{2}} \frac{n_i B(\psi'_i - \psi'_{i-1}) - n_{i-1}B(\psi'_{i-1} - \psi'_i)}{\Delta} \tag{54}$$

This means that the equation we needs to solve turns into:

$$qD_{i+\frac{1}{2}} \frac{n_{i+1}B(\psi'_{i+1} - \psi'_i) - n_i B(\psi'_i - \psi'_{i+1})}{\Delta^2} - \\ qD_{i-\frac{1}{2}} \frac{n_i B(\psi'_i - \psi'_{i-1}) - n_{i-1}B(\psi'_{i-1} - \psi'_i)}{\Delta^2} = q(R_i - G_i) \tag{55}$$

After the equation is divided by q, The left side of the equation can be sorted in terms of order of n:

$$\frac{D_{i-\frac{1}{2}} B(\psi'_{i-1} - \psi'_i)}{\Delta^2} n_{i-1} - \frac{D_{i+\frac{1}{2}} B(\psi'_i - \psi'_{i+1}) + D_{i-\frac{1}{2}} B(\psi'_i - \psi'_{i-1})}{\Delta^2} n_i + \\ \frac{D_{i+\frac{1}{2}} B(\psi'_{i+1} - \psi'_i)}{\Delta^2} n_{i+1} = R_i - G_i \tag{56}$$

For LU Decomposition

$$b(i) = \frac{D_{i-\frac{1}{2}} B(\psi'_{i-1} - \psi'_i)}{\Delta^2} \tag{57}$$

$$a(i) = -\frac{D_{i+\frac{1}{2}} B(\psi'_i - \psi'_{i+1}) + D_{i-\frac{1}{2}} B(\psi'_i - \psi'_{i-1})}{\Delta^2} \tag{58}$$

$$c(i) = \frac{D_{i+\frac{1}{2}} B(\psi'_{i+1} - \psi'_i)}{\Delta^2} \tag{59}$$

$$x(i) = n(i) \tag{60}$$

$$f(i) = R_{SRH} = \frac{n_i(p(i)n(i)) - 1)}{\tau_p[n(i) + 1] + \tau_n[p(i) + 1]} \tag{61}$$

However, we treat n without the factor of the intrinsic concentration and only as a function of psi. This means the generation rate can be divided by ni for the calculation of n

D can also be approximated as an average of the closest values:

$$D_{i+\frac{1}{2}} = \frac{D_i + D_{i+1}}{2} \tag{62}$$

$$D_{i-\frac{1}{2}} = \frac{D_i + D_{i-1}}{2} \tag{63}$$

For LU Decomposition

$$b(i) = \frac{D_i + D_{i-1}}{2} \frac{B(\psi'_{i-1} - \psi'_i)}{\Delta^2} \tag{64}$$

$$a(i) = -\left(\frac{D_i + D_{i+1}}{2} \frac{B(\psi'_i - \psi'_{i+1})}{\Delta^2} + \frac{D_i + D_{i-1}}{2} \frac{B(\psi'_i - \psi'_{i-1})}{\Delta^2}\right) \tag{65}$$

$$c(i) = \frac{D_i + D_{i+1}}{2} \frac{B(\psi'_{i+1} - \psi'_i)}{\Delta^2} \tag{66}$$

$$x(i) = n(i) \tag{67}$$

$$f(i) = R_{SRH} = \frac{n_i(p(i)n(i)) - 1)}{\tau_p[n(i) + 1] + \tau_n[p(i) + 1]} \tag{68}$$

12 Sharfetter-Gummel [3, p.158-159]

These equations are changed from the book to fit the 1D Scheme. Also variables have been changed to make sense in context to the rest of these notes.

12.1 Electrons

$$D_{i+\frac{1}{2}}\frac{n_{i+1}B(\psi'_{i+1}-\psi'_i)-n_iB(\psi'_i-\psi'_{i+1})}{\Delta^2}- \\ D_{i-\frac{1}{2}}\frac{n_iB(\psi'_i-\psi'_{i-1})-n_{i-1}B(\psi'_{i-1}-\psi'_i)}{\Delta^2}=R_i \quad (69)$$

$$n_{i+1}\frac{D_{i+\frac{1}{2}}B(\psi'_{i+1}-\psi'_i)}{\Delta^2}-n_i\frac{D_{i+\frac{1}{2}}B(\psi'_i-\psi'_{i+1})}{\Delta^2}- \\ n_i\frac{D_{i-\frac{1}{2}}B(\psi'_i-\psi'_{i-1})}{\Delta^2}+n_{i-1}\frac{D_{i-\frac{1}{2}}B(\psi'_{i-1}-\psi'_i)}{\Delta^2}=R_i \quad (70)$$

$$n_{i+1}\frac{D_{i+\frac{1}{2}}B(\psi'_{i+1}-\psi'_i)}{\Delta^2}-n_i\frac{D_{i+\frac{1}{2}}B(\psi'_i-\psi'_{i+1})+D_{i-\frac{1}{2}}B(\psi'_i-\psi'_{i-1})}{\Delta^2}+ \\ n_{i-1}\frac{D_{i-\frac{1}{2}}B(\psi'_{i-1}-\psi'_i)}{\Delta^2}=R_i \quad (71)$$

$$a(i)=-\frac{D_{i+\frac{1}{2}}B(\psi'_i-\psi'_{i+1})+D_{i-\frac{1}{2}}B(\psi'_i-\psi'_{i-1})}{\Delta^2} \quad (72)$$

$$b(i)=\frac{D_{i-\frac{1}{2}}B(\psi'_{i-1}-\psi'_i)}{\Delta^2} \quad (73)$$

$$c(i)=\frac{D_{i+\frac{1}{2}}B(\psi'_{i+1}-\psi'_i)}{\Delta^2} \quad (74)$$

$$f(i)=R_i \quad (75)$$

12.2 Holes

$$D_{i+\frac{1}{2}}\frac{p_{i+1}B(\psi'_i-\psi'_{i+1})-p_iB(\psi'_{i+1}-\psi'_i)}{\Delta^2}- \\ D_{i-\frac{1}{2}}\frac{p_iB(\psi'_{i-1}-\psi'_i)-p_{i-1}B(\psi'_i-\psi'_{i-1})}{\Delta^2}=R_i \quad (76)$$

$$p_{i+1}\frac{D_{i+\frac{1}{2}}B(\psi'_i-\psi'_{i+1})}{\Delta^2}-p_i\frac{D_{i+\frac{1}{2}}B(\psi'_{i+1}-\psi'_i)}{\Delta^2}- \\ p_i\frac{D_{i-\frac{1}{2}}B(\psi'_{i-1}-\psi'_i)}{\Delta^2}+p_{i-1}\frac{D_{i-\frac{1}{2}}B(\psi'_i-\psi'_{i-1})}{\Delta^2}=R_i \quad (77)$$

$$p_{i+1}\frac{D_{i+\frac{1}{2}}B(\psi'_i-\psi'_{i+1})}{\Delta^2}-p_i\frac{D_{i+\frac{1}{2}}B(\psi'_{i+1}-\psi'_i)+D_{i-\frac{1}{2}}B(\psi'_{i-1}-\psi'_i)}{\Delta^2}+ \\ p_{i-1}\frac{D_{i-\frac{1}{2}}B(\psi'_i-\psi'_{i-1})}{\Delta^2}=R_i \quad (78)$$

$$a(i)=-\frac{D_{i+\frac{1}{2}}B(\psi'_{i+1}-\psi'_i)+D_{i-\frac{1}{2}}B(\psi'_{i-1}-\psi'_i)}{\Delta^2} \quad (79)$$

$$b(i)=\frac{D_{i-\frac{1}{2}}B(\psi'_i-\psi'_{i-1})}{\Delta^2} \quad (80)$$

$$c(i)=\frac{D_{i+\frac{1}{2}}B(\psi'_i-\psi'_{i+1})}{\Delta^2} \quad (81)$$

$$f(i)=R_i \quad (82)$$

13 Discretized Current Equations

Using the discretized current equations eq. 52 and eq. 54 and the discretized diffusion averages eq. 62 and eq. 63:

$$J_{i+\frac{1}{2}} = q\frac{D_i + D_{i+1}}{2}\frac{n_{i+1}B(\psi'_{i+1} - \psi'_i) - n_iB(\psi'_i - \psi'_{i+1})}{\Delta} \tag{83}$$

$$J_{i-\frac{1}{2}} = q\frac{D_i + D_{i-1}}{2}\frac{n_iB(\psi'_i - \psi'_{i-1}) - n_{i-1}B(\psi'_{i-1} - \psi'_i)}{\Delta} \tag{84}$$

$$J_i = \frac{J_{i-\frac{1}{2}} + J_{i+\frac{1}{2}}}{2} \tag{85}$$

$$\begin{aligned} J_i = \frac{q}{2\Delta}[\frac{D_i + D_{i+1}}{2}(n_{i+1}B(\psi'_{i+1} - \psi'_i) - n_iB(\psi'_i - \psi'_{i+1}))+ \\ \frac{D_i + D_{i-1}}{2}(n_iB(\psi'_i - \psi'_{i-1}) - n_{i-1}B(\psi'_{i-1} - \psi'_i))] \end{aligned} \tag{86}$$

$$\begin{aligned} J_i = \frac{qn_i}{2\Delta}[\frac{D_i + D_{i+1}}{2}(n(i+1)B(\psi'_{i+1} - \psi'_i) - n(i)B(\psi'_i - \psi'_{i+1}))+ \\ \frac{D_i + D_{i-1}}{2}(n(i)B(\psi'_i - \psi'_{i-1}) - n(i-1)B(\psi'_{i-1} - \psi'_i))] \end{aligned} \tag{87}$$

14 Bernoulli Function Implementation [3, p.169]

Bernoulli Function:

$$B(x) = \frac{x}{exp(x) - 1}$$

Suggested Implementation:

$$B(x) = \begin{cases} -x & x \leq x1 \\ \frac{x}{exp(x)-1} & x1 \leq x \leq x2 \\ 1 - \frac{x}{2} & x2 \leq x \leq x3 \\ \frac{xexp(-x)}{1-exp(-x)} & x3 \leq x \leq x4 \\ xexp(-x) & x4 \leq x \leq x5 \\ 0 & x5 \leq x \end{cases}$$

Constants Discretely Defined by:

$$exp(x1) - 1 = -1 \tag{88}$$

$$x2/(exp(x2) - 1) = 1 - (x2/2), x2 < 0 \tag{89}$$

$$1 - (x3/2) = x3exp(-x3)/(1 - exp(-x3)), x3 > 0 \tag{90}$$

$$1 - exp(-x4) = 1 \tag{91}$$

$$exp(-x5) = 0 \tag{92}$$

15 Equilibrium Results

References

[1] ATLAS User's Manual Device Simulation Software Volume I, 1998.

[2] Robert F. Pierret. *Semiconductor Device Fundamentals*. Addison-Wesley Publishing Company, 1996.

[3] Siegfried Selberherr. *Analysis and Simulation of Semiconductor Devices*. Springer-Verlag, New York, 1984.

[4] Dragica Vasileska and Stephen M Goodnick. *Computational Electronics*. Morgan & Claypool Publishers, 2006.

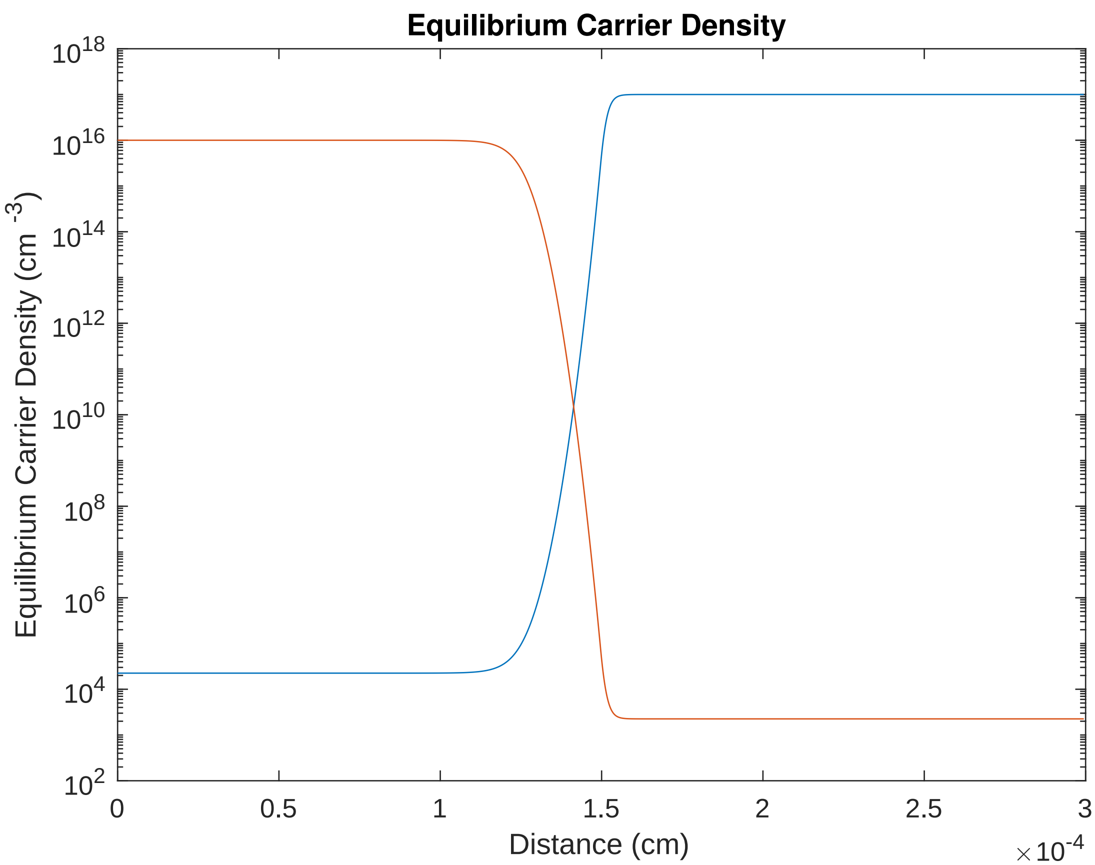

Figure 1: Equilibrium Carrier Density

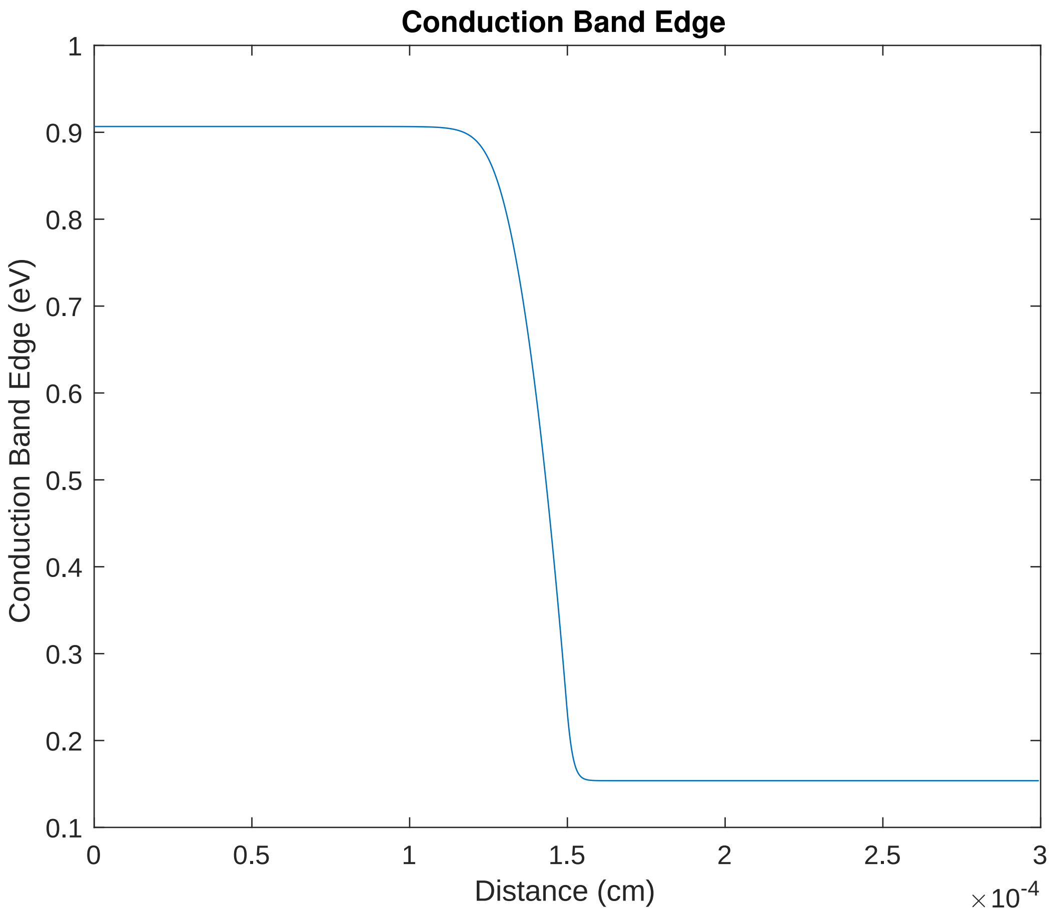

Figure 2: Equilibrium Carrier Density

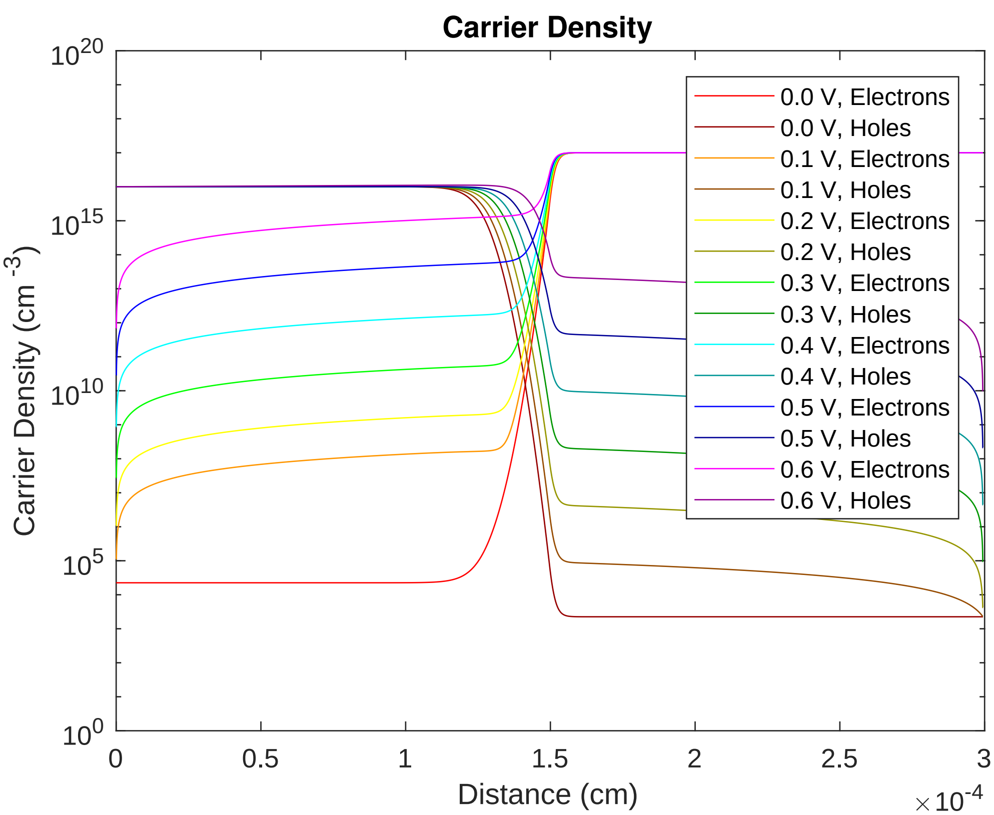

Figure 3: Carrier Density in a p-n junction by voltage steps of 0.1 V.

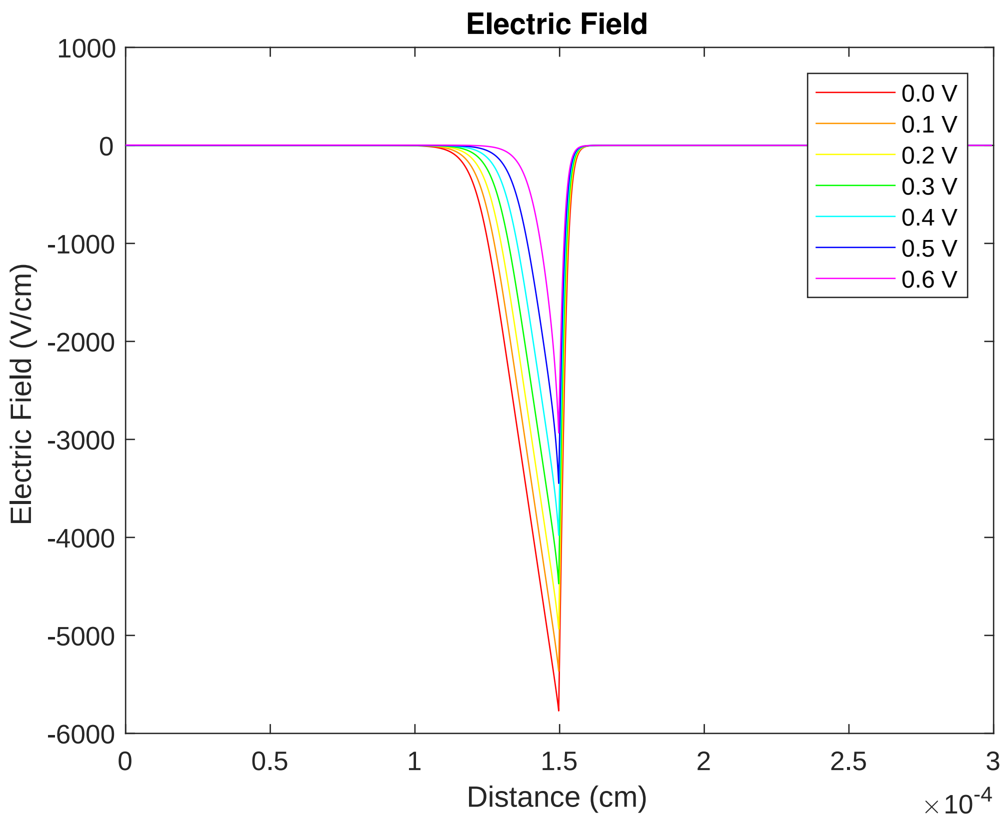

Figure 4: Electric Field in a p-n junction by voltage steps of 0.1 V.

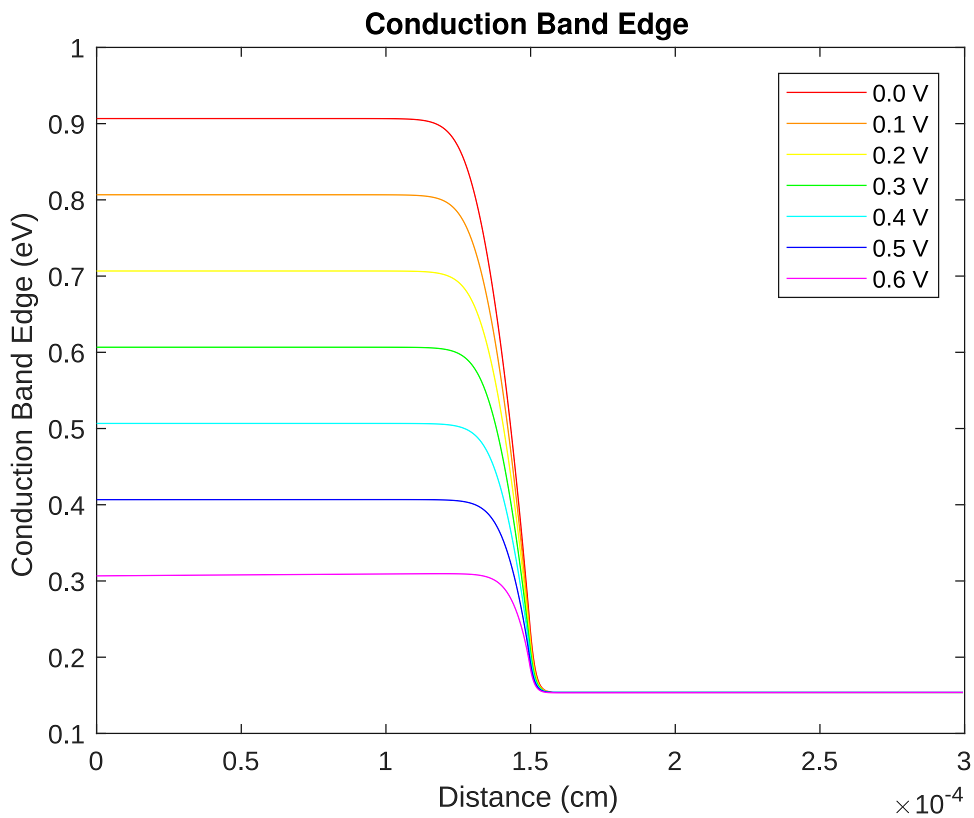

Figure 5: Conduction Band in a p-n junction by voltage steps of 0.1 V.

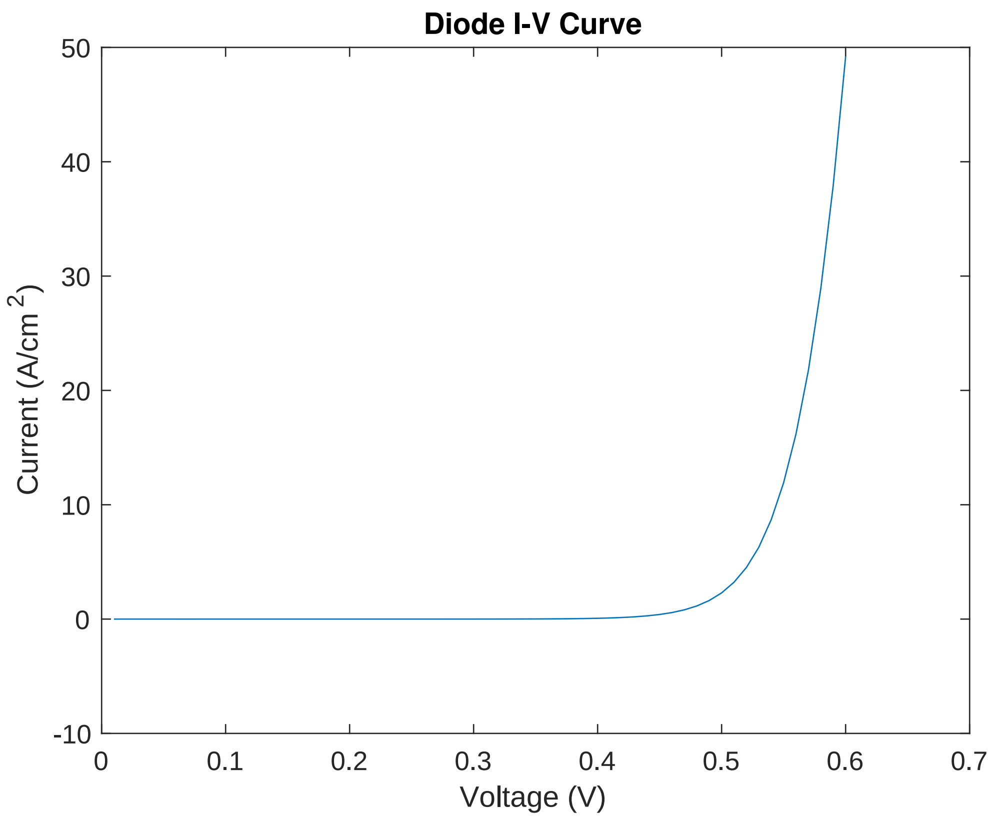

Figure 6: Diode IV Curve - Magnitude seems high?