Semiconductor Solver

Gaurav Somani

CeNSE, IISc

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Introduction

- Like most of the physical systems, semiconductor system variables can be tied in a set of partial differential equations
- Due to non-linearity of equations, space variation of electric potential and current-voltage relationship in semiconductors is non-linear
- Can't apply ohm's law
- Analytical approximations can't always be made justifiably
- Numerical methods come to the rescue

Fundamental Equations:Equilibrium

Equilibrium implies no electric current flow and constant fermi level.
Poisson equation:

$$\nabla^2\psi = -\frac{q(N_D - N_A + p - n)}{\epsilon} \tag{1}$$

Carrier Statistics:

$$n = N_C F_{1/2}\left(\frac{q(\psi - \psi_i)}{k_B T}\right)$$
$$p = N_V F_{1/2}\left(\frac{-q(E_g + \psi - \psi_i)}{k_B T}\right) \tag{2}$$

where F_j represents complete Fermi-Dirac integral of order j

Fundamental Equations:Non-equilibrium steady state

Conservation equation: Recombination rate is rate at which carriers combine per unit volume per unit time.

$$R - G = \frac{\vec{\nabla}.\vec{J_n}}{q} = -\frac{\vec{\nabla}.\vec{J_p}}{q} \tag{3}$$

Drift-Diffusion:

$$\begin{aligned} \vec{J_n} &= -qn\mu_n \nabla \phi_n \\ \vec{J_p} &= -qn\mu_p \nabla \phi_p \end{aligned} \tag{4}$$

SRH Recombination:

$$R = \frac{pn - n_i^2}{\tau_n(p + n_i) + \tau_p(n + n_i)} \tag{5}$$

G is generation rate (generally, due to optical excitation)

Domain geometry

- 2-D Cylindrically symmetric (r and z)
- 2-D Rectangular with reflection symmetry (x and y)
- 1-D (Rectangular) (x)
- 1-D (Circular) (r)
- 1-D (Spherical) (r)

Boundary conditions for well-defined solution

- Equilibrium : Potential boundary conditions and normal electric field boundary lead to unique solution for poisson equation
- Non-equilibrium steady state : Dirichlet boundary conditions are physically known (voltage bias and contact nature)
- Vertical boundaries have reflecting boundary conditions

Normalisation

- Conversion of physical quantities to dimensionless form by dividing by suitable physical values

$$
\begin{aligned}
V_T = \frac{k_B T}{q}; L_D = \sqrt{\frac{\epsilon V_T}{q n_i}} \\
E_0 = \frac{V_T}{L_D}; J_o = \frac{q \mu_n n_i V_T}{L_D} \\
t_0 = \frac{\epsilon}{q \mu_n n_i}; R_o = \frac{n_i}{t_0}
\end{aligned} \tag{6}
$$

Leads to much simpler equations

Linearisation and Discretisation

- Linearisation : Linearisation of non-linear PDE about current solution
  Non-linearity in poisson equation due to carrier statistics linearised using derivative wrt potential

$$\nabla^2\psi = r + \psi(N_C F_{-1/2}(\bar{\Phi} - \psi_i) + N_V F_{-1/2}(\psi_i - E_g - \bar{\Phi})) \tag{7}$$

  where ψ is the change in the potential approximation
- Discretisation : Discretisation of linearised PDE to set of linear equations
  For poisson equation, discretised laplacian is used for different geometries
  For conservative quantities, numerically integration over control area about each mesh point is performed.
- Linearised equations when discretised lead to matrix equations

Input for equilibrium

- Set up mesh and contact nature (boundary conditions)
- Define doping profile
- Solve for equilibrium potential and carrier density
- Plot results

Input for biased system

- Set up mesh and contact nature (boundary conditions)
- Define doping profile and carrier lifetimes
- Define generation rate (default is 0 everywhere)
- Set bias sweep range
- Solve for potential, carrier density and current density
- Plot results

Setting up mesh and boundary conditions

- Mesh generation : User inputs the critical points and mesh spacing. Automated non-uniform smooth mesh is generated by geometric interpolation. Mesh spacing should be less than L_D (debye length) to resolve fine features. Also, non-uniform mesh allows having good condition number. Mesh should be fine at junctions.
- Boundary conditions : Electrical boundary conditions in user input converted to physical boundary conditions in terms of solution variables

Initial guess

- **Equilibrium Poisson Equation**: Based on analytical solution after removing coupling between neighbouring mesh points
  Based on the reasoning that device can be constructed by putting pieces of semiconductor together
- **Biased non-equilibrium steady state**: For initial bias, solution at equilibrium is used as initial guess

Numerical methods

- Gauss-Laguerre quadrature for numerical evaluation of FD integral

$$F_j(x) = \frac{1}{\Gamma(j+1)} \int_0^\infty w_j(t) \frac{1}{e^{-t} + e^{-x}} dt$$
$$= \frac{1}{\Gamma(j+1)} \int_0^\infty w_j(t) g(t) dt$$

$$\textit{where } w_j(t) = t^j e^{-t} \textit{ and } g(t) = \frac{1}{e^{-t} + e^{-x}}.$$

- SOR + Multi-grid
- Alternate direction implicit method
- Tridiagonal matrix algorithm
- Relaxation method
- Newton-Raphson method
- Banded matrix algorithms

SOR + multigrid

- SOR (iterative method) is used for equilibrium calculation as good initial guess is available
- Potential has low frequency modes
- SOR on fine mesh (more points) takes a large number of iterations to resolve
- SOR with multi-grid resolves lower frequency modes at coarser mesh
- Mesh is coarsened recursively until mesh becomes coarse enough so solution becomes computationally cheap
- Solution at coarser mesh is interpolated to finer mesh as initial guess

ADI

- 1D problem leads to tridiagonal matrix with fast solution
- ADI by splitting the laplacian along orthogonal dimensions
- Faster than SOR + multigrid in most cases

Relaxation for coupled PDE at steady state

- Coupled PDE system solved by solving one PDE at a time considering only one solution variable
- Robust for low bias and insensitive to poor guess
- Slow(linear) convergence

Newton's method for coupled PDE

- Linearised description of coupled PDE system in terms of 3N variables is calculated
- Newton's method is applied to Jacobian to calculate next approximate solution
- Fast(Quadratic) convergence
- Highly sensitive to initial guess
- Used in combination with relaxation method to ensure robustness and speed

Faster implementation

- Red-black scheme of ordering variables for vectorized implementation of SOR
- Pre-computation of Fermi-Dirac integral and use of cubic splines to approximate it at runtime
- Alternate row and alternate column iterations for vectorized ADI
- Reordering of variables of coupled PDE for steady state to form banded matrix
- Combination of relaxation and newton-raphson methods
- Pre-computation of Laplacian stencil

Problems related to numerical solution

- Noisy current density
  Solution : Under steady state reverse bias, currents become very low and exponent calculation of very close numbers lead to loss of numerical precision. So, instead of 64 bits float, 80 bits long double is used. It makes solution reliable and can speed up convergence in most cases.
- High coupling between coupled PDE at high bias under steady state leading to non-convergence or very slow convergence
  Solution : Jacobian of coupled system is used to linearise the system. Then, newton-raphson method is applied to linearised system in $3N$ variables with reordered variables leading to banded matrix which speeds up the convergence

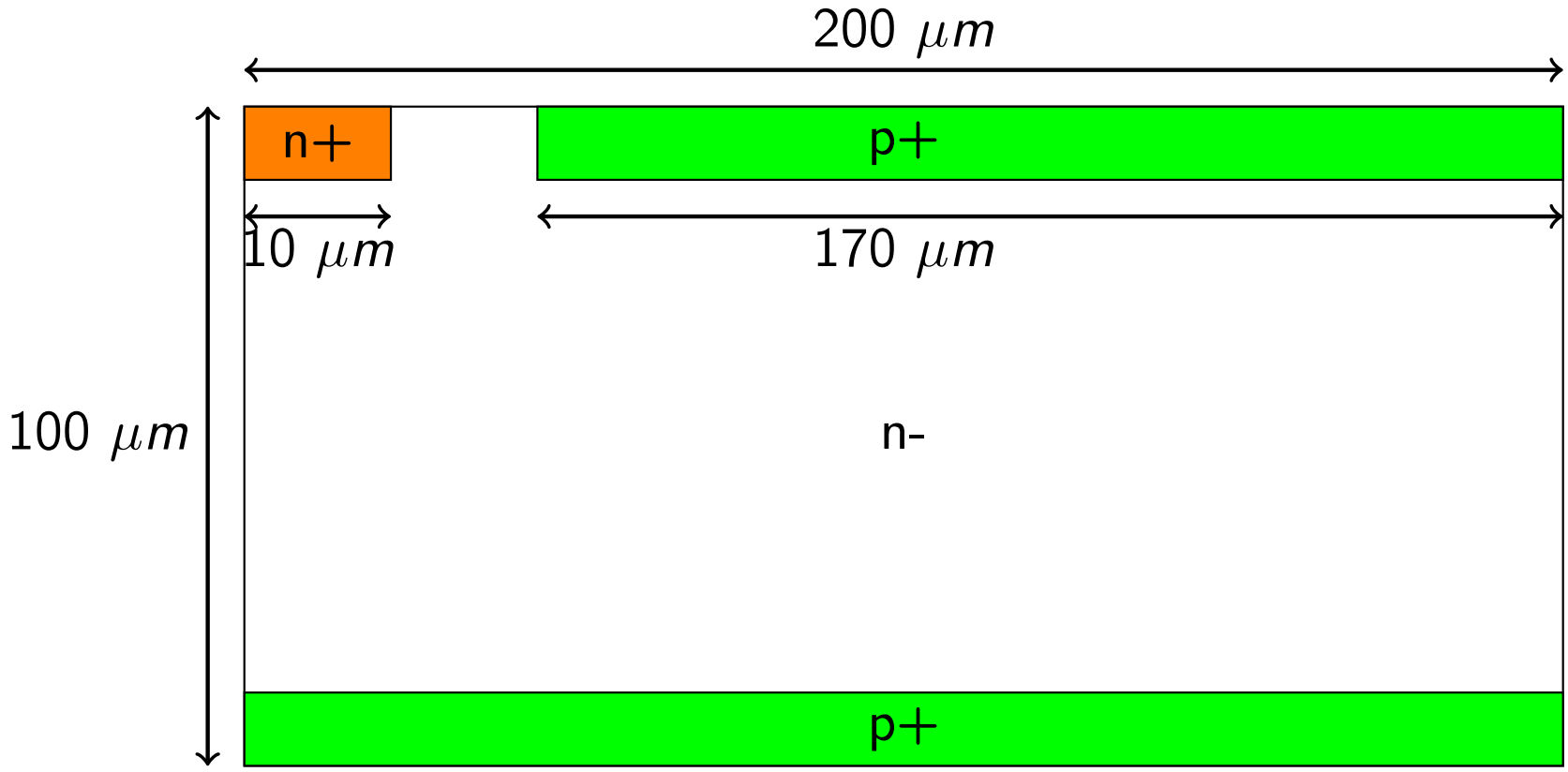


Figure 1: Input structure (SDD)

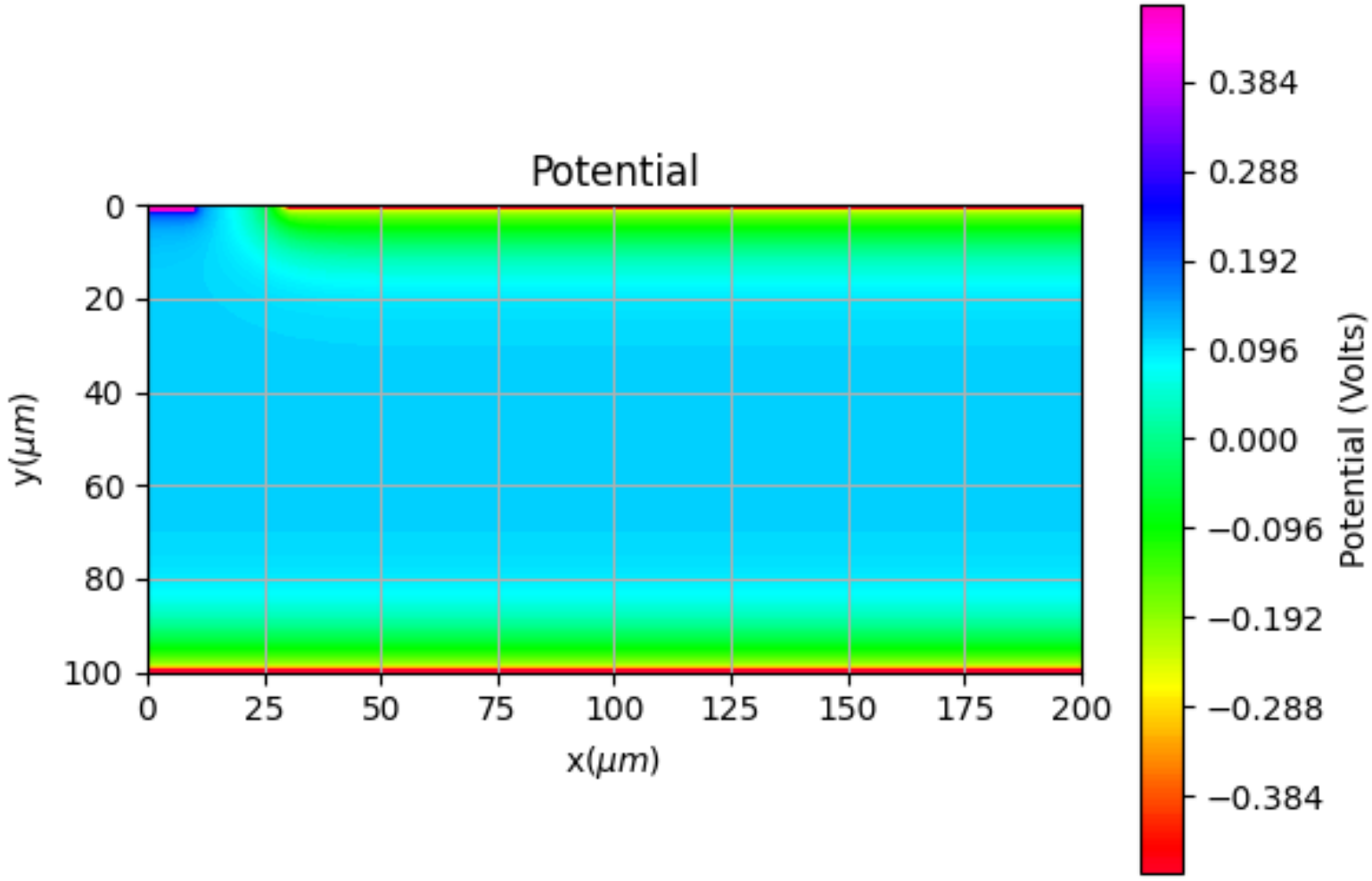


Figure 2: Potential contour plot showing potential variation near the junction by this solver

Commercial simulator used to compare results is SILVACO ATLAS.

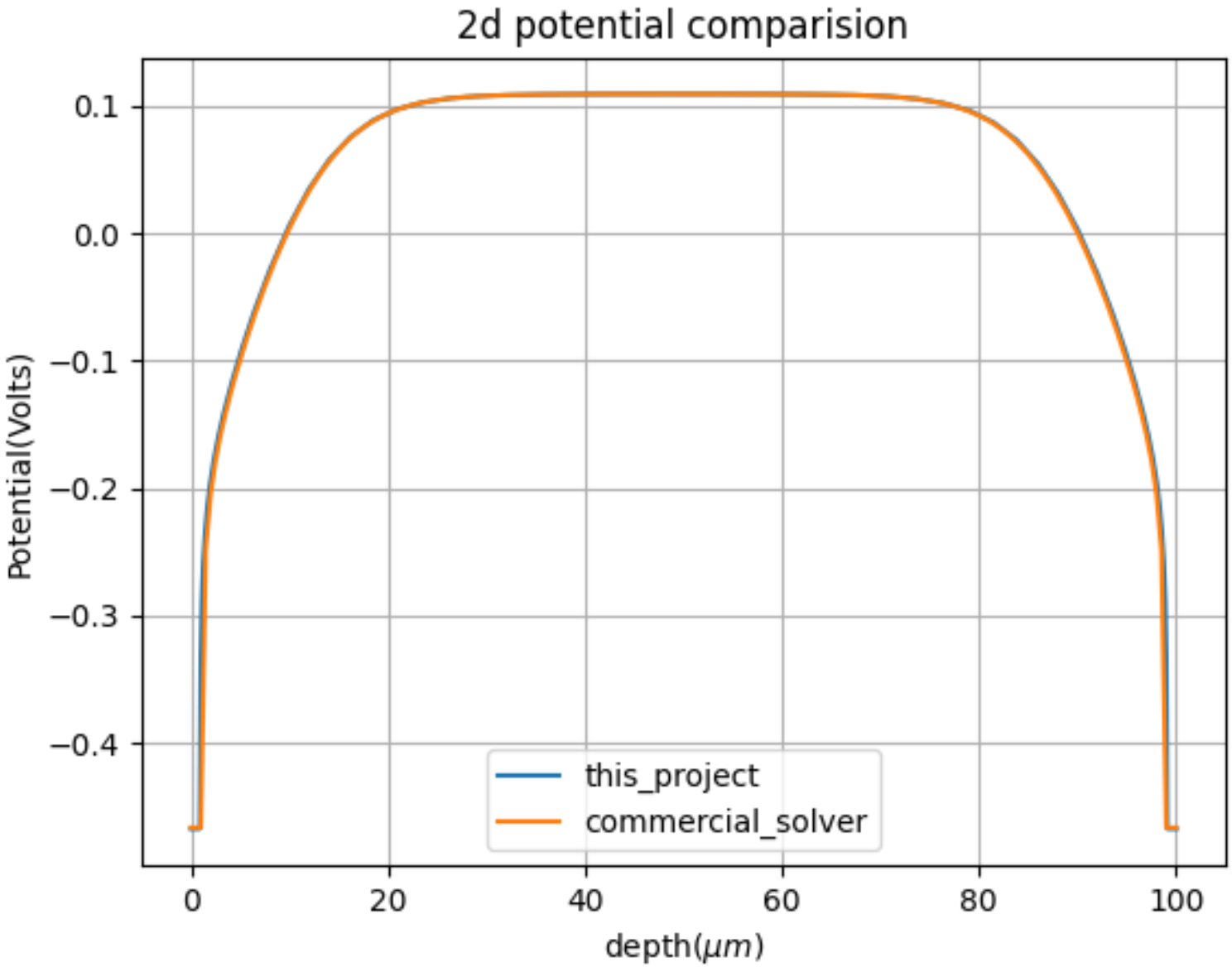


Figure 3: Potential section at $r = 41.2\mu m$

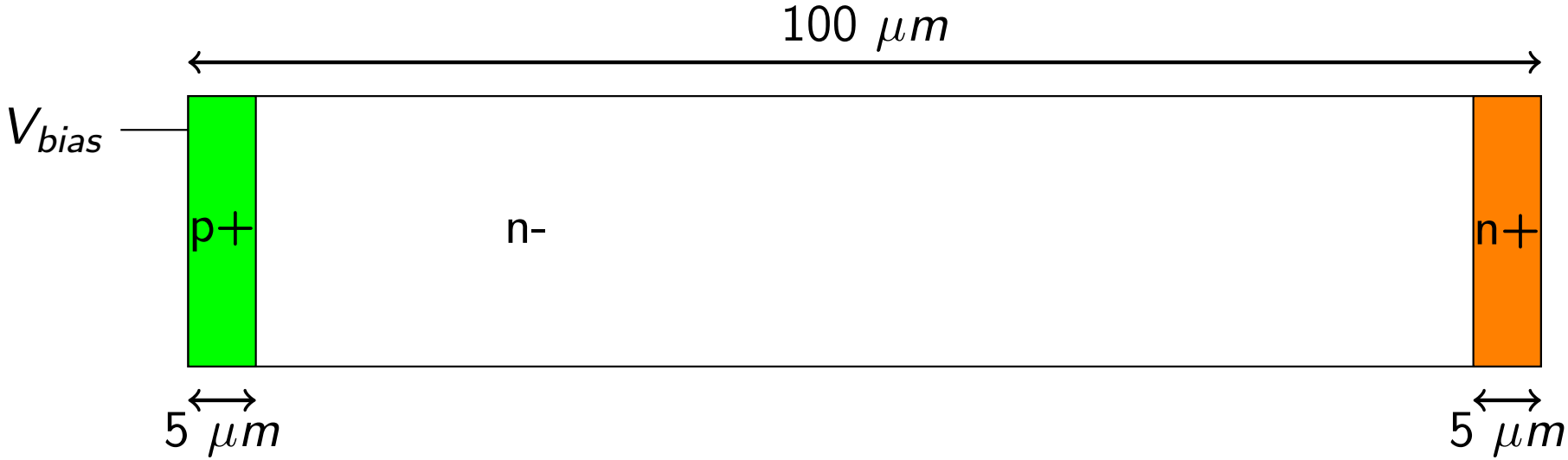


Figure 4: PIN diode

Results : Potential at equilibrium

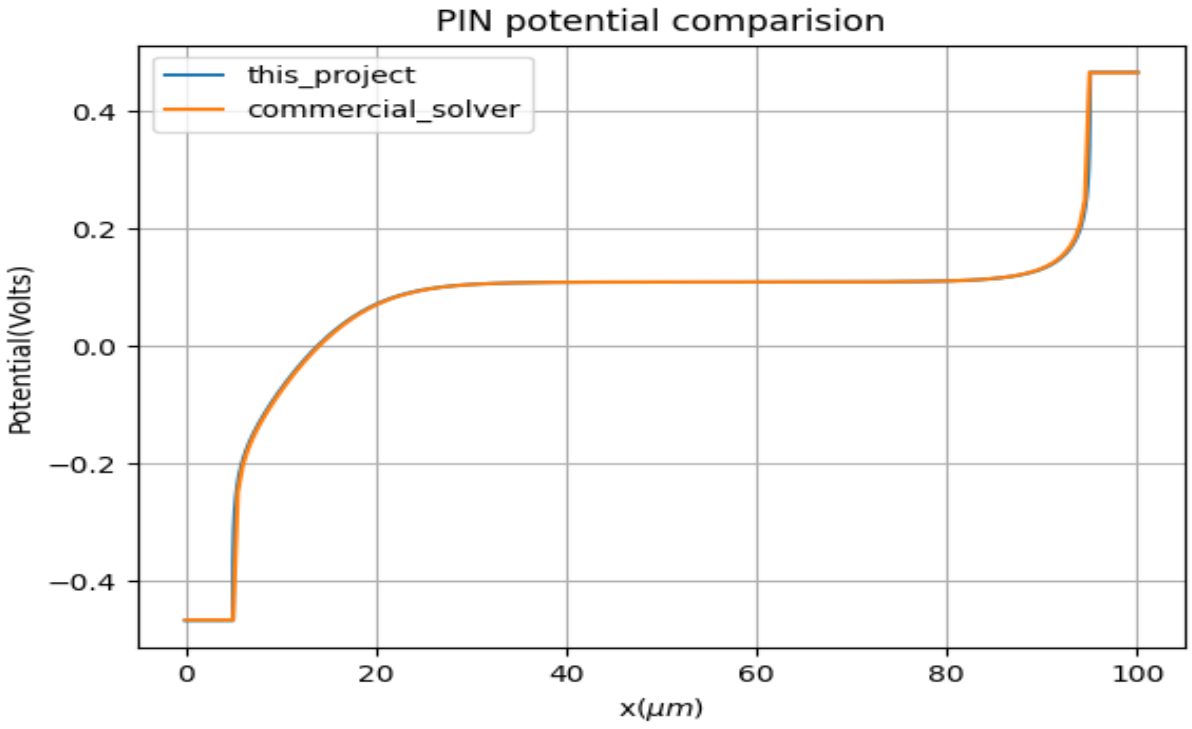


Figure 5: Potential barrier at equilibrium

$$W_{dep} = \sqrt{\frac{2\epsilon_{Si} V_{bi}}{qN}}$$

which is about $25\mu m$

Results : Potential in a biased pn-junction

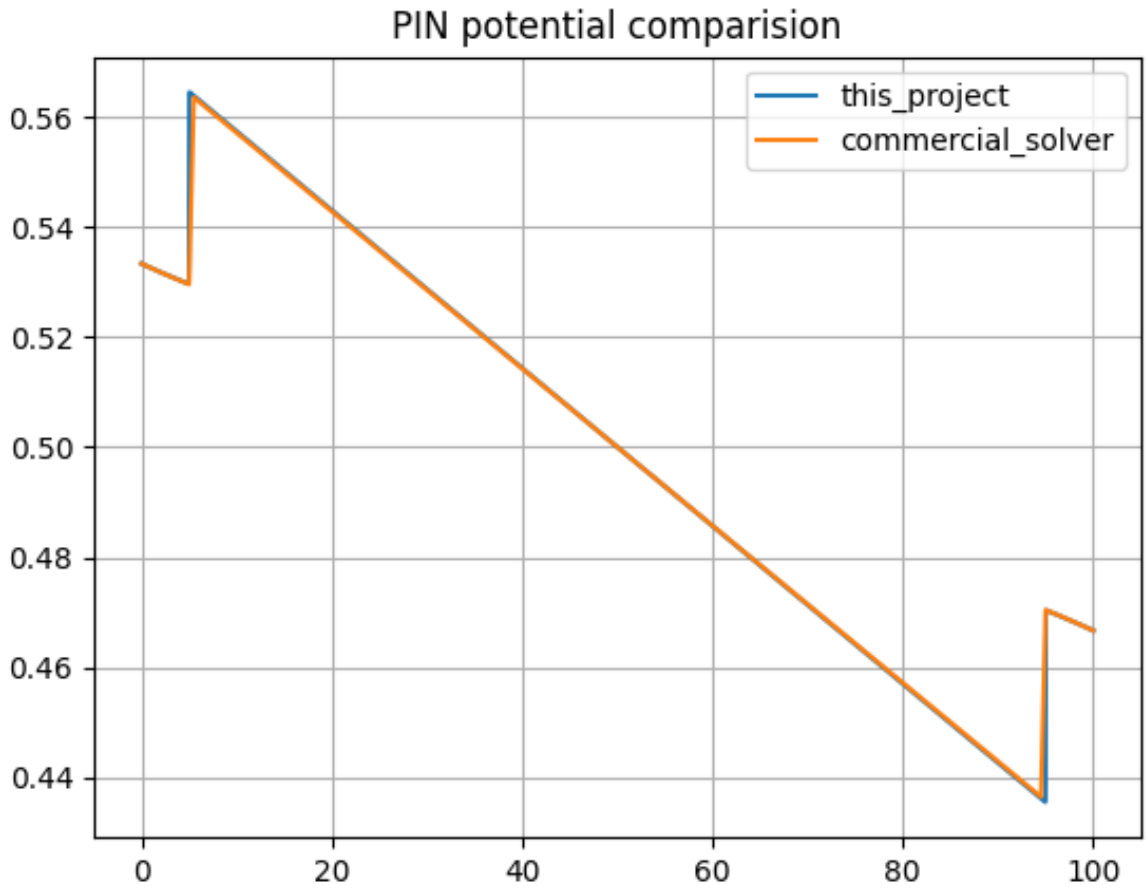


Figure 6: Potential barrier lowered in forward bias

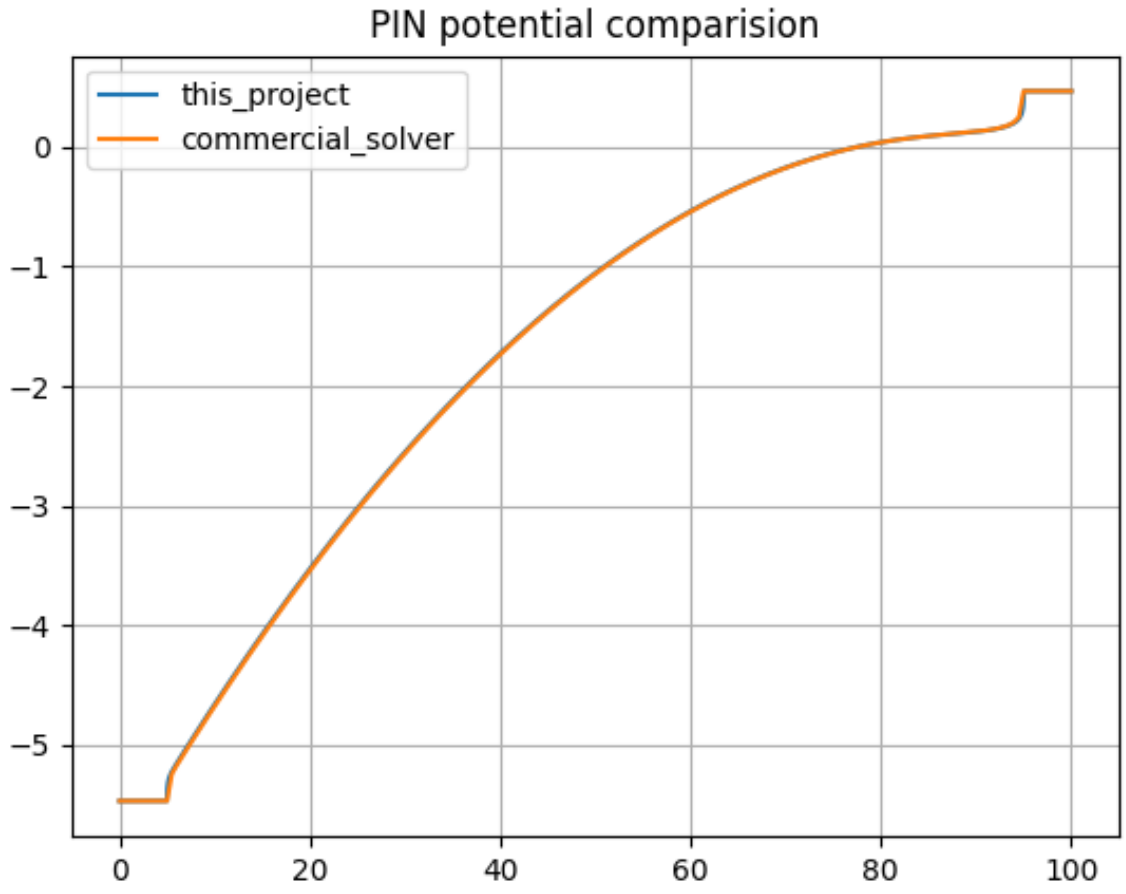
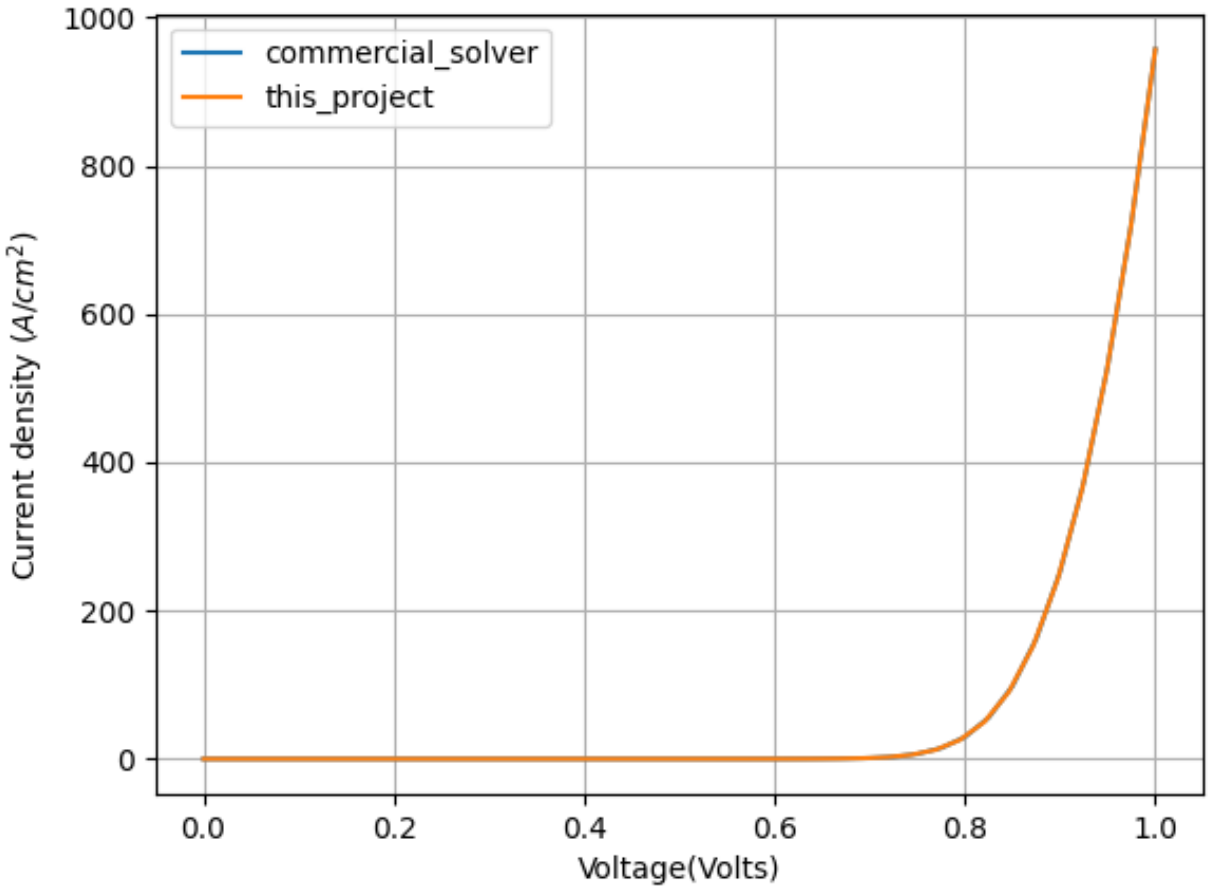


Figure 7: Potential barrier increased in reverse bias

Results: Current density in a biased p-njunction

Current density for an ideal p-n junction diode can be approximated by :

$$J = J_0(e^{qV/k_BT} - 1)$$



Results: Current density in a biased pn-junction

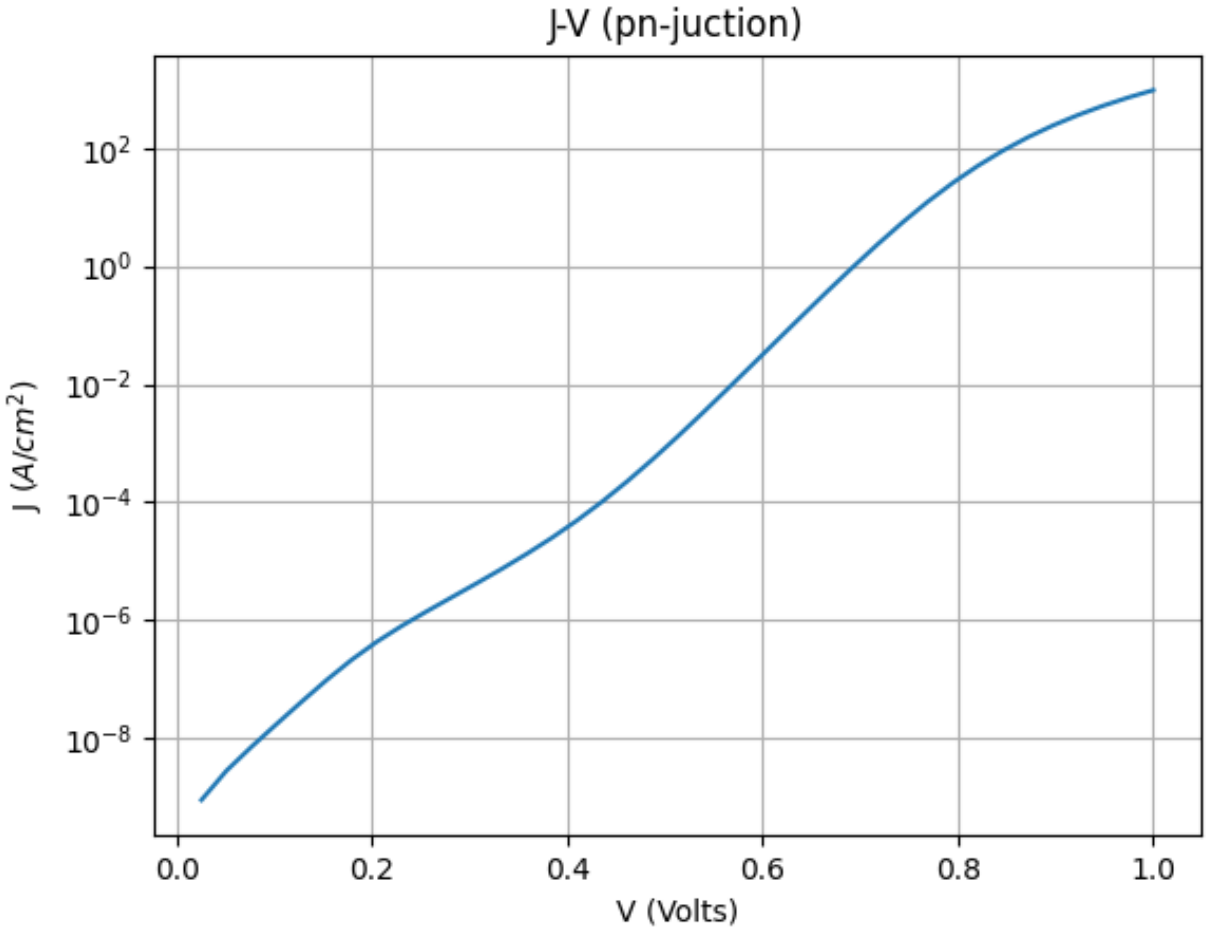


Figure 9: Current density in forward bias(Logarithmic scale) (compare with 10)

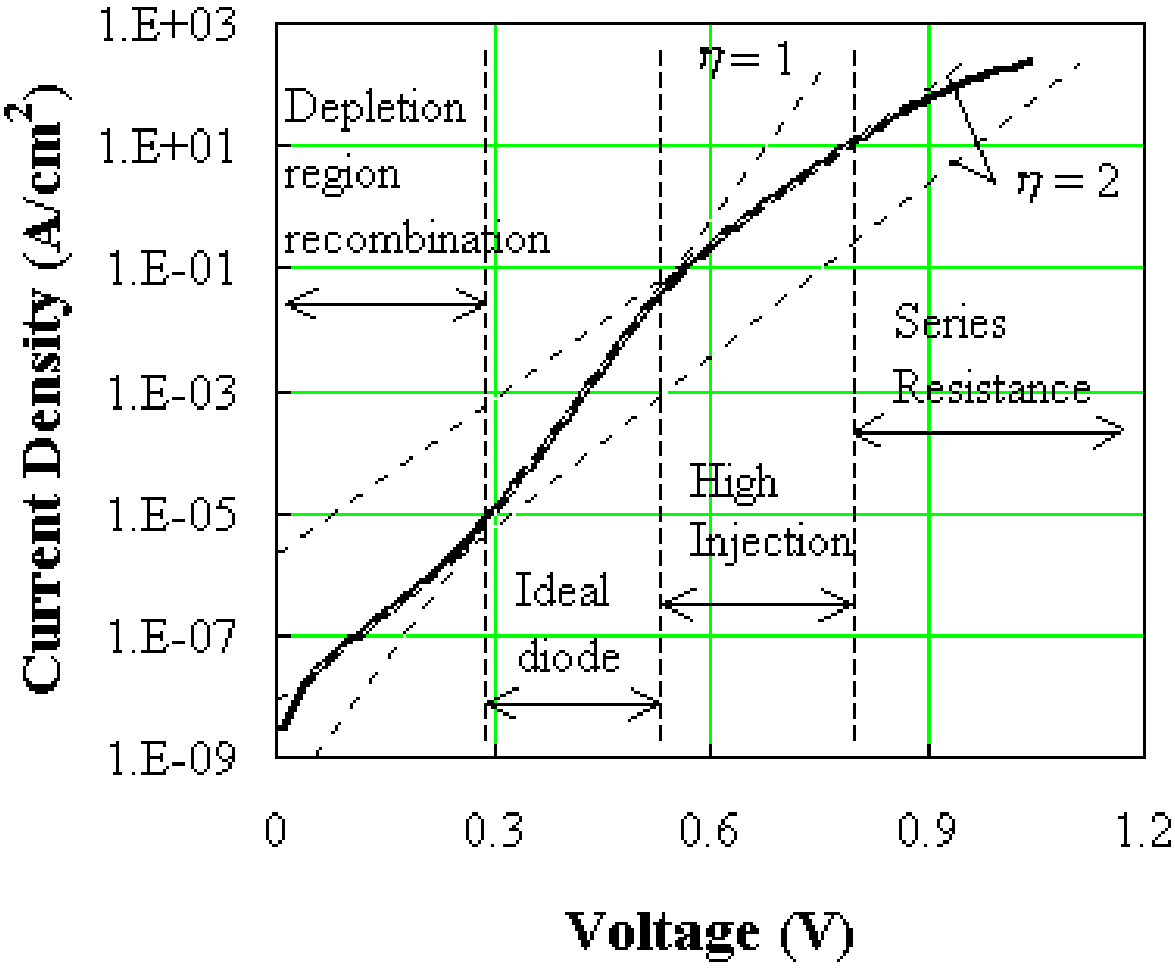


Figure 10: Image taken from Principles of Semiconductor Devices,B. Van Zeghbroeck, 2011

$$J_{gen} = qn_i \frac{W_D}{\tau_n + \tau_p} \approx 10^{-8} A/cm^2$$

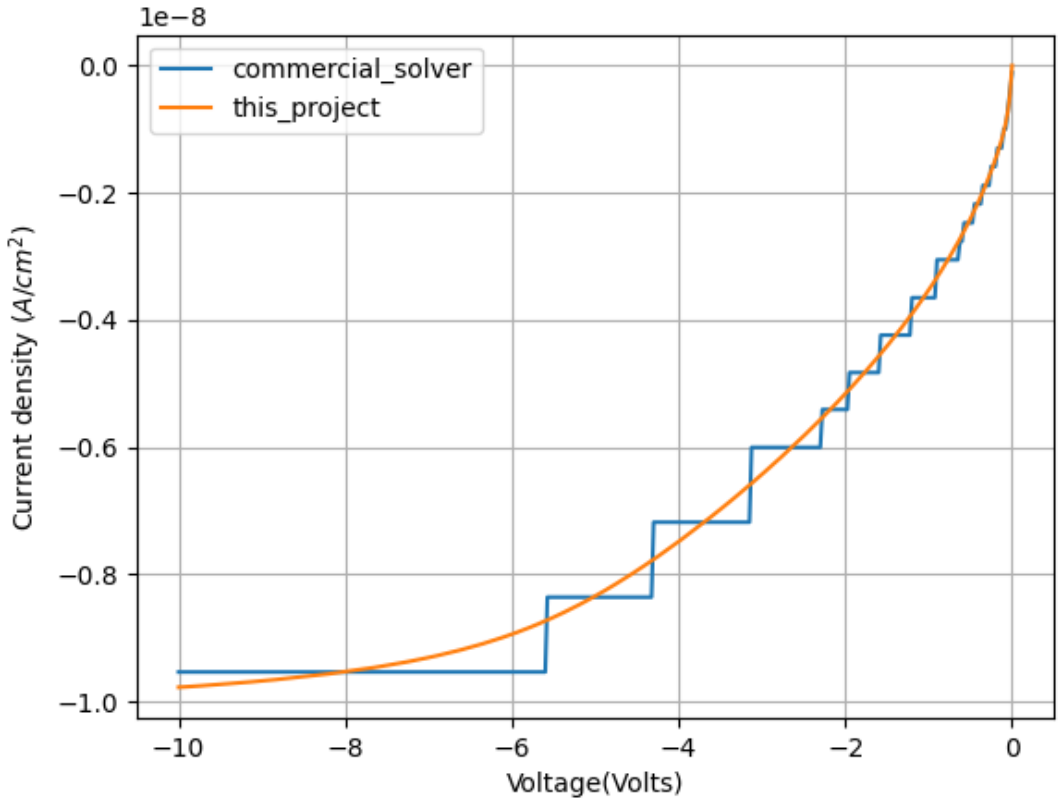


Figure 11: Current density in reverse biased PIN diode due to generation happening in depletion region (See noisy current density with commercial simulator due to lower precision of 64 bits compared to 80 bits used in this solver)