Computational Microelectronics L16

Sung-Min Hong

smhong@gist.ac.kr

Semiconductor Device Simulation Laboratory, GIST

Continuity equation

Electron and hole densities

- How can we calculate those quantities?
  - In the nonlinear Poisson equation, we assume

$$n = n_{int} \exp\left(\frac{\phi}{V_T}\right)$$

$$p = n_{int} \exp\left(-\frac{\phi}{V_T}\right)$$

  - Note that the above expressions are valid only at equilibrium.
- At nonequilibrium cases, we need a general method.
  - Solve additional equations for them.

Continuity equations

- Continuity equations are appropriate ones.

$$\frac{\partial c}{\partial t} = -\nabla \cdot \mathbf{F}_c$$

  - Here, c is either n (the electron density) or p (the hole density).
  - (We have seen it before.)
  - The flux, $\mathbf{F}_c$, is related with the current density, $\mathbf{J}_c$.

$$\mathbf{J}_c = \pm q \mathbf{F}_c$$

Upper sign for holes, lower sign for electrons

Current density

- Sum of drift and diffusion terms
  - For electrons,

$$\mathbf{J}_n = -q\mu_n n \nabla\phi + qD_n \nabla n$$

  - For holes,

$$\mathbf{J}_p = -q\mu_p p \nabla\phi - qD_p \nabla p$$

- Similarity with the diffusion simulation?
  - Yes, we have seen a similar expression before.
  - At that time, we introduced additional approximations.

Derivation

- How can we derive the continuity equation?
  - It can be rigorously derived from the Boltzmann transport equation.
  - The distribution function, $f(\mathbf{r}, \mathbf{k}, t)$, satisfies

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla_r f + \frac{\mathbf{F}}{\hbar} \cdot \nabla_k f = \hat{S}$$

- How can we derive the current density?
  - Well, it can be also derived from the Boltzmann transport equation.

Electron continuity at a steady-state

- No time derivative
  - The electron current density becomes divergenceless (solenoidal).

$$\frac{1}{q}\nabla \cdot \mathbf{J}_n = \frac{\partial n}{\partial t} = 0$$

Steady-state

  - The electron current density reads: (Einstein relation)

$$\mathbf{J}_n = qD_n\left(\nabla n - \frac{1}{V_T} n \nabla \phi\right)$$

  - 1D case, J_n

$$\frac{dJ_n}{dx} = 0$$

$$J_n = qD_n\left(\frac{dn}{dx} - \frac{1}{V_T} n \frac{d\phi}{dx}\right)$$

Discretization

- Integration from $x_{i-0.5}$ to $x_{i+0.5}$
  - Just like the Poisson equation,

$$\int_{x_{i-0.5}}^{x_{i+0.5}} \frac{dJ_n}{dx} dx = J_n(x_{i+0.5}) - J_n(x_{i-0.5}) = 0$$

  - How about the electron current density?

$$J_n(x_{i+0.5}) = qD_n \left(\left.\frac{dn}{dx}\right|_{x_{i+0.5}} - \frac{1}{V_T} n \left.\frac{d\phi}{dx}\right|_{x_{i+0.5}} \right)$$

Finite difference

- Recall that

$$\left.\frac{d\phi}{dx}\right|_{x_{i+0.5}} = \frac{\phi_{i+1} - \phi_i}{x_{i+1} - x_i}$$

- Electron current density

$$J_n(x_{i+0.5}) = \frac{qD_n}{x_{i+1} - x_i}\left[(n_{i+1} - n_i) - \frac{1}{V_T}\frac{n_{i+1} + n_i}{2}(\phi_{i+1} - \phi_i)\right]$$

  - A similar expression for $J_n(x_{i-0.5})$

- Hole current density

$$J_p(x_{i+0.5}) = -\frac{qD_p}{x_{i+1} - x_i}\left[(p_{i+1} - p_i) + \frac{1}{V_T}\frac{p_{i+1} + p_i}{2}(\phi_{i+1} - \phi_i)\right]$$

Jacobian

- From the following expression,

$$J_n(x_{i+0.5}) = \frac{qD_n}{x_{i+1} - x_i}\left[(n_{i+1} - n_i) - \frac{1}{V_T}\frac{n_{i+1} + n_i}{2}(\phi_{i+1} - \phi_i)\right]$$

  – Components of Jacobian matrix are given as

$$\frac{\partial J_n(x_{i+0.5})}{\partial n_{i+1}} = \frac{qD_n}{x_{i+1} - x_i}\left[1 - \frac{\phi_{i+1} - \phi_i}{2V_T}\right]$$

$$\frac{\partial J_n(x_{i+0.5})}{\partial n_i} = \frac{qD_n}{x_{i+1} - x_i}\left[-1 - \frac{\phi_{i+1} - \phi_i}{2V_T}\right]$$

$$\frac{\partial J_n(x_{i+0.5})}{\partial \phi_{i+1}} = \frac{qD_n}{x_{i+1} - x_i}\left[-\frac{n_{i+1} + n_i}{2V_T}\right]$$

$$\frac{\partial J_n(x_{i+0.5})}{\partial \phi_i} = \frac{qD_n}{x_{i+1} - x_i}\left[\frac{n_{i+1} + n_i}{2V_T}\right]$$

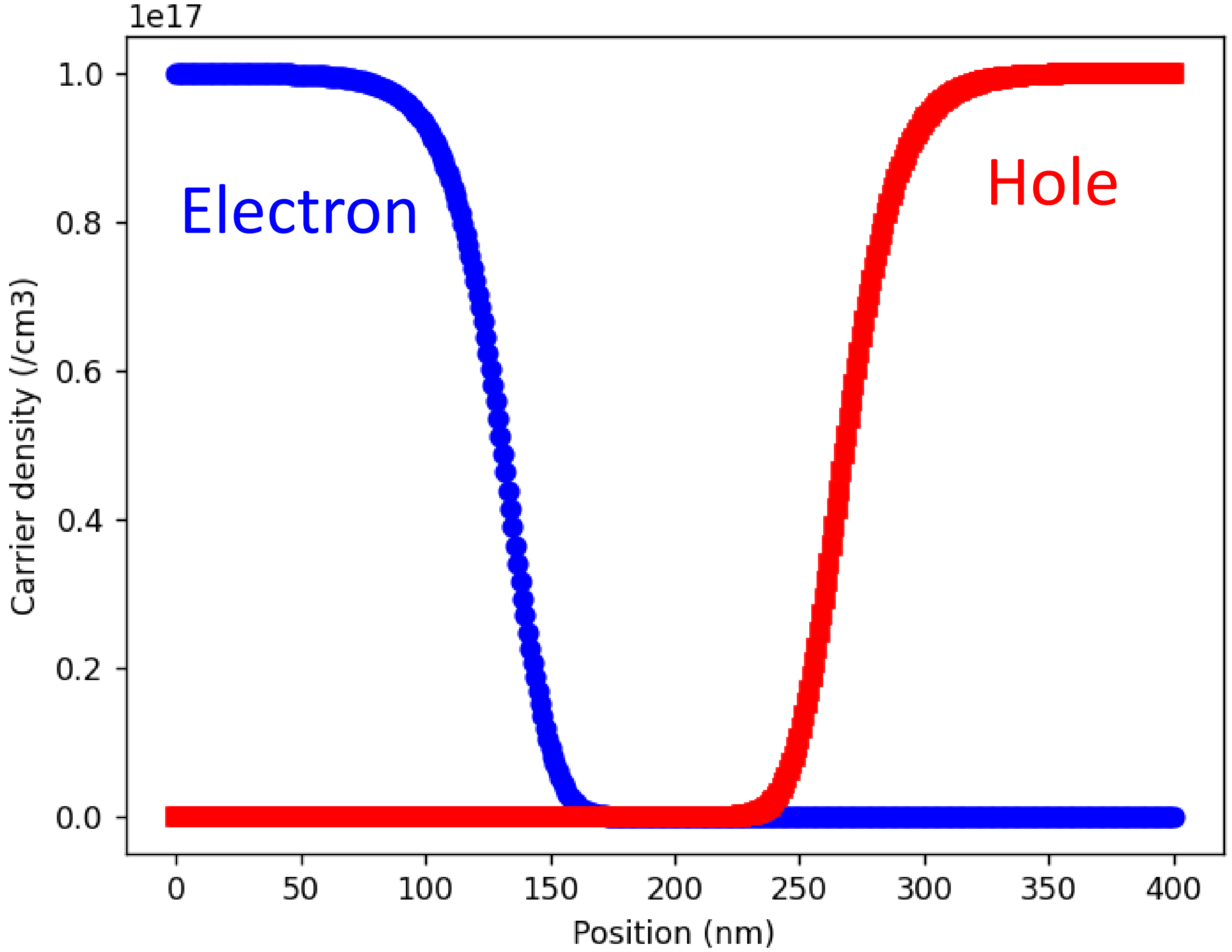
Arranging variables & B. C.

- Three variables (ϕ, n, and p) at each vertex
  - $3i$ for potential, $3i + 1$ for electrons, $3i$ +2 for holes
  - Carrier densities are fixed at two boundaries.

$$\begin{bmatrix} \text{Poisson} \\ \text{Electron continuity} \\ \text{Hole continuity} \\ \text{Poisson} \\ \text{Electron continuity} \\ \text{Hole continuity} \\ \ldots \end{bmatrix} \text{X} \begin{bmatrix} \delta\phi \\ \delta n \\ \delta p \\ \delta\phi \\ \delta n \\ \delta p \\ \vdots \end{bmatrix} = \begin{bmatrix} r_\phi \\ r_n \\ r_p \\ r_\phi \\ r_n \\ r_p \\ \vdots \end{bmatrix}$$

Equilibrium

- $N_D = N_A = 10^{17}$ cm^{-3}. 1-nm spacing



Bias ramping

Bias ramping

- We start from the equilibrium solution at 0 V
  - Increase the anode voltage (Forward)
  - Decrease the anode voltage (Reverse)
  - Boundary condition for the cathode contact

$$r_0 = \phi(x_0) - \phi_0\left(N_{dop}^{+}(x_0)\right)$$
$$A_{0,0} = 1$$

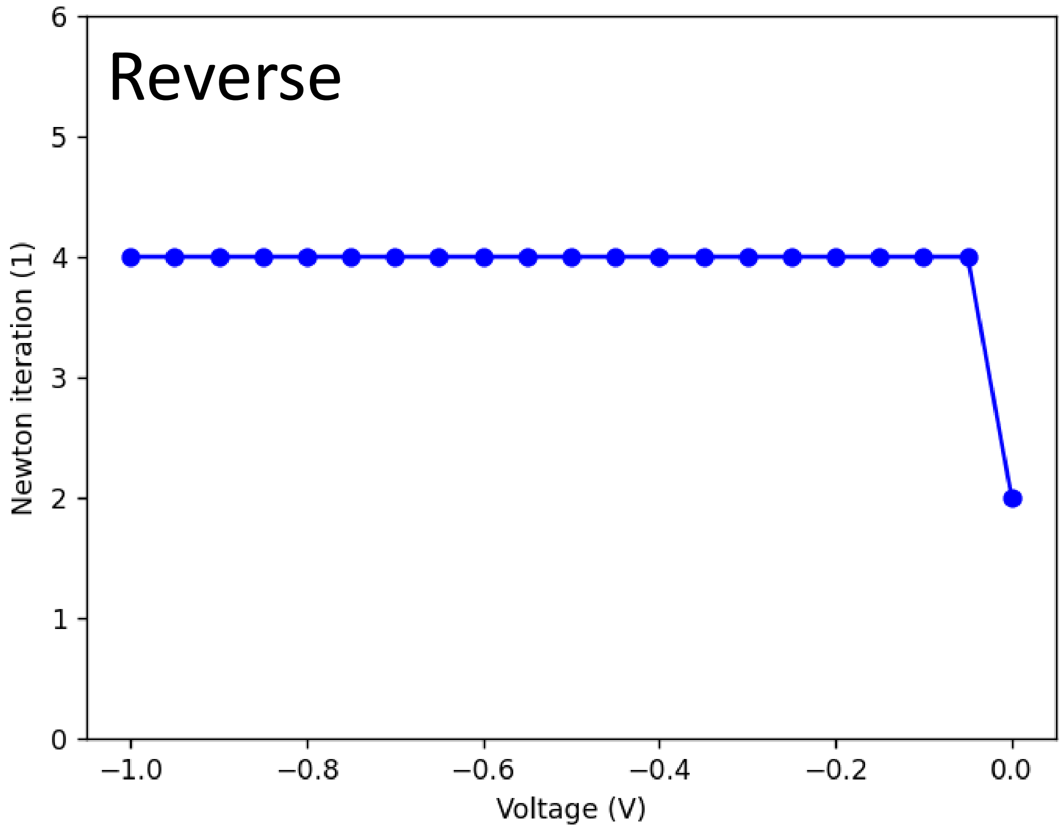
  - Boundary condition for the anode contact

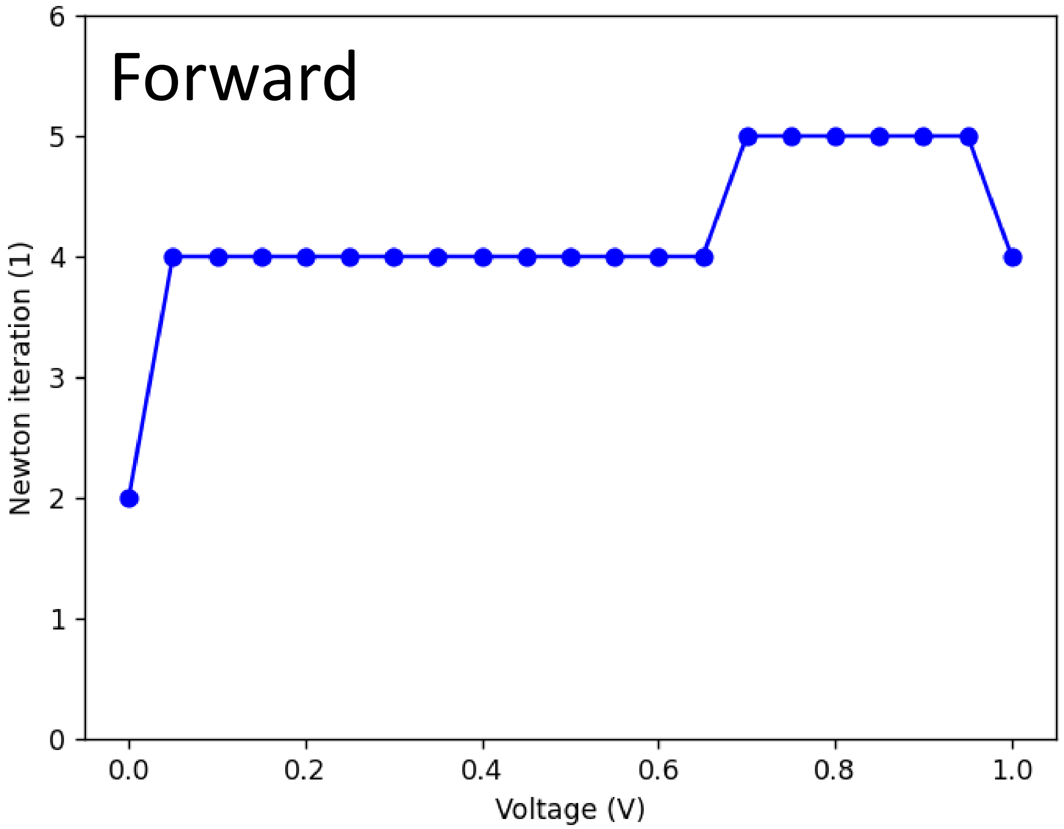
$$r_{3N} = \phi(x_N) - \phi_0\left(N_{dop}^{+}(x_N)\right) - V_{anode}$$
$$A_{3N,3N} = 1$$

Equilibrium potential

Number of Newton iterations

- Convergence criterion of 10^{-10} V
  - We need 4~5 iterations at each bias point.





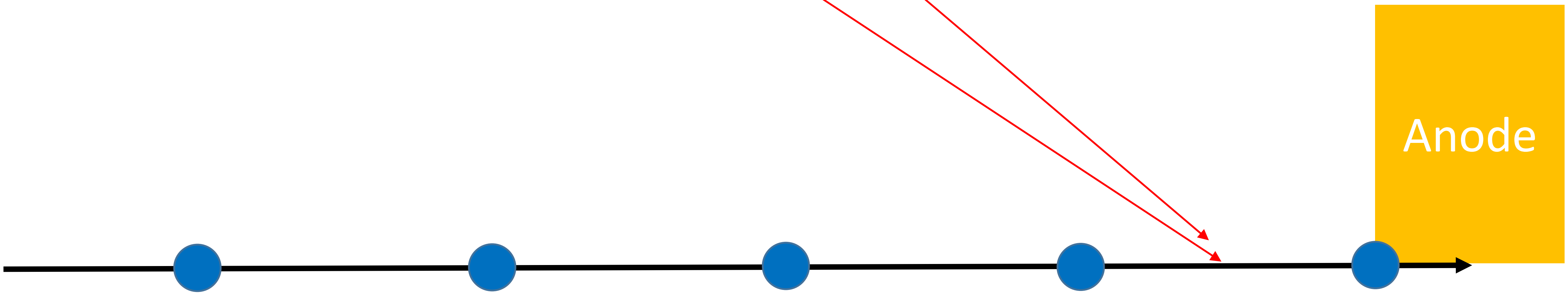
Terminal current

- In a steady-state,

$$I_{terminal} = -\int_{terminal\ area} (\mathbf{J}_p + \mathbf{J}_n) \cdot d\mathbf{a}$$

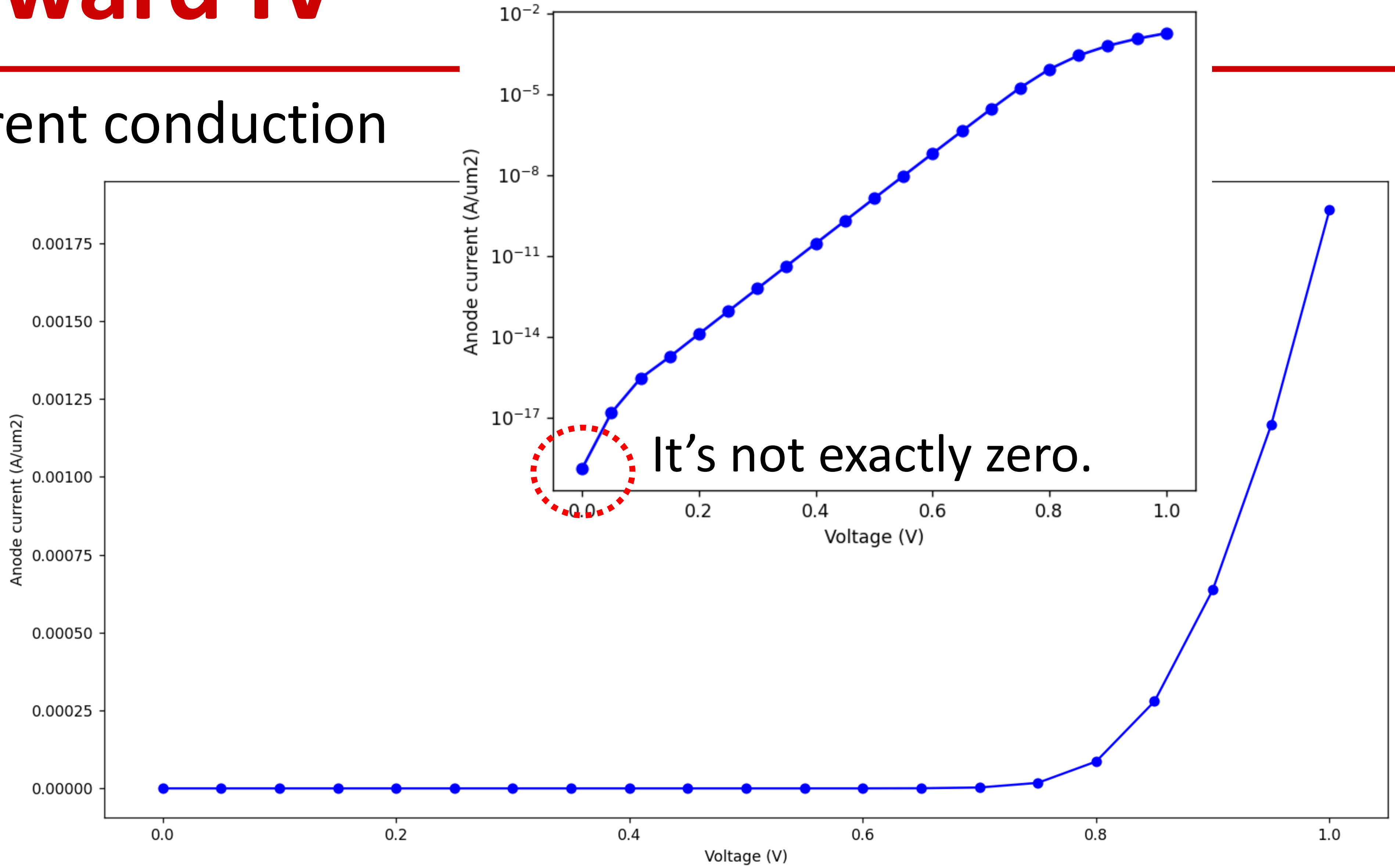
- In a 1D structure, it is very simple.
  - Sum of current densities at the edge connected to the terminal

$$I_{anode} = -(J_p + J_n)A$$



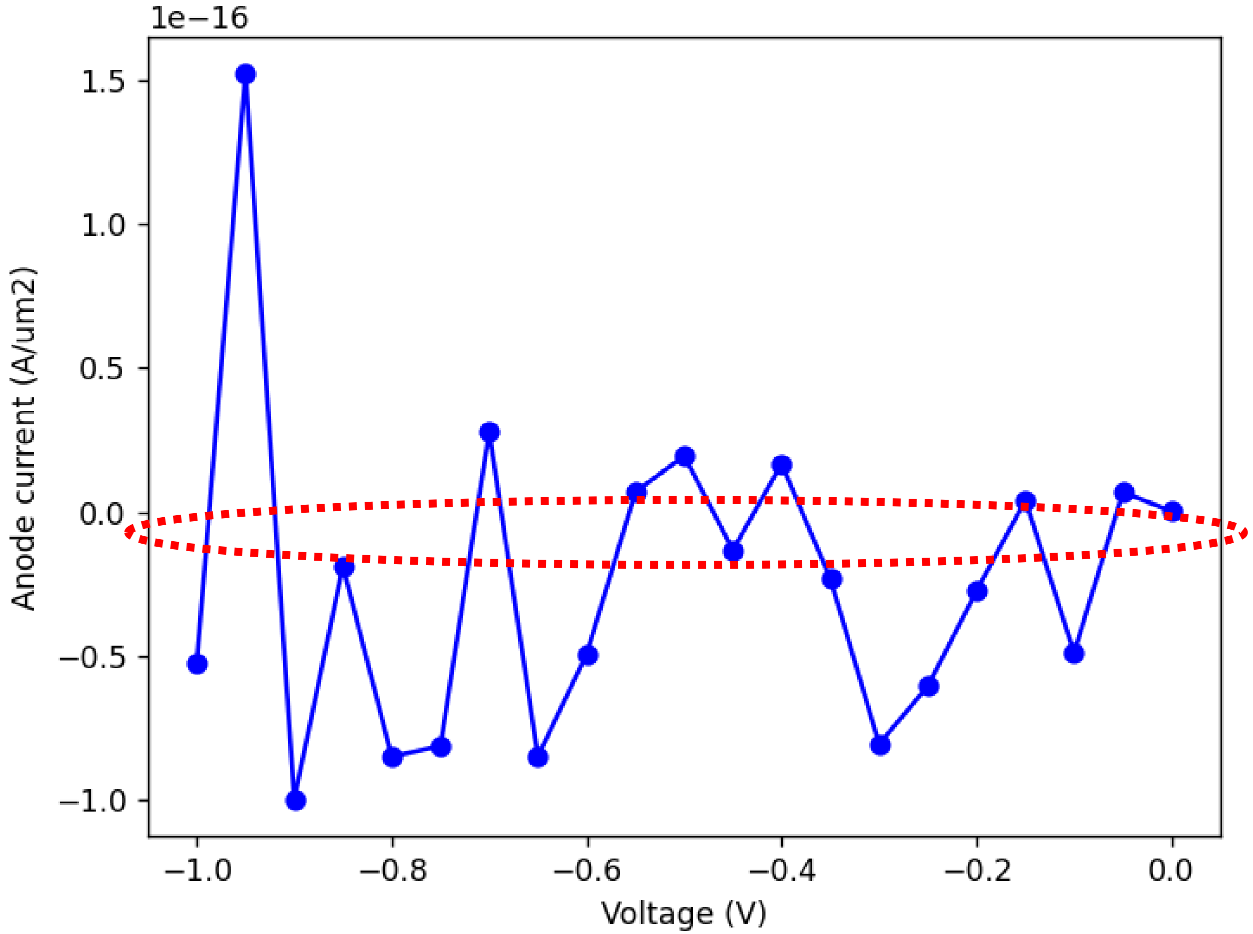
Forward IV

- Current conduction



Reverse IV

- No current conduction



Homework#16

- Due: AM08:00, November 14
- Problem#1
  - Calculate the IV characteristics of the PN junction considered in this lecture. Assume that μ_n = 1417 cm^2/V sec and μ_p = 470.5 cm^2/V sec.

Thank you for your attention!