Computational Microelectronics
Lecture 16 Continuity Equation

Sung-Min Hong (smhong@gist.ac.kr)
Semiconductor Device Simulation Laboratory
School of Electrical Engineering and Computer Science
Gwangju Institute of Science and Technology

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, $f(\mathbf{r}, \mathbf{k}, r)$, 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).

$$\frac{1}{q}\nabla \cdot \mathbf{J}_n = \frac{\partial n}{\partial t} = 0 \longleftarrow \text{Steady-state}$$

  - 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

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

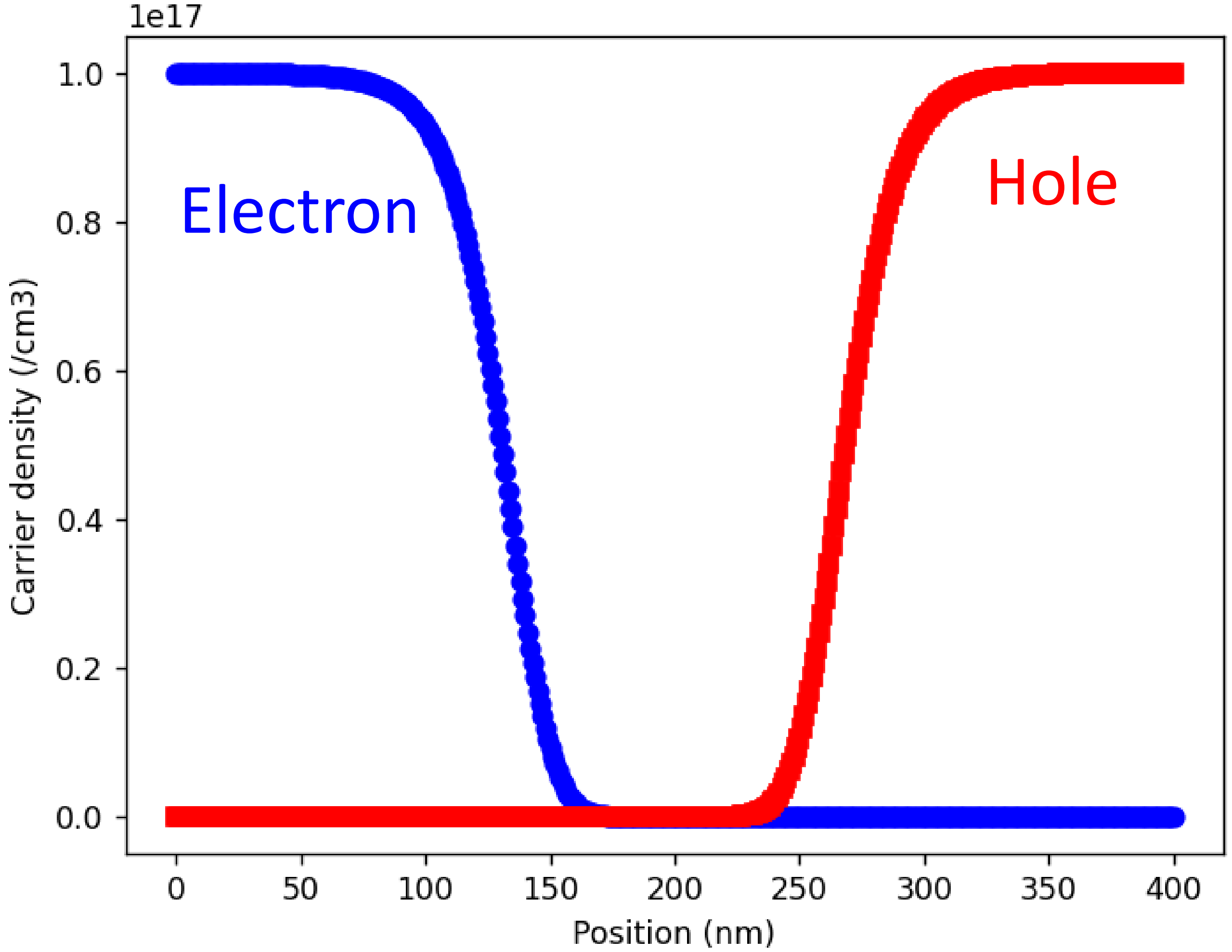
$$\frac{\partial J_n(x_{i+0.5})}{\partial n_i} = \frac{qD_n}{x_{i+1} - x_i}\left[-1 - \frac{\phi_{i+1} - \phi_i}{2V_T}\right]$$

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

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

Equilibrium

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



Thank you!