

# Computational Microelectronics

## Lecture 6 Diffusion

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# Diffusion – Electric Field

# Drift

- Up to now, we have considered only the diffusion term.

- The flux was written as ( $\# \text{ cm}^{-2} \text{ sec}^{-1}$ )

$$\mathbf{F}_C = -D\nabla C$$

- If we consider a charged dopant ion, the drift should be also considered.

$$\mathbf{F}_C = -D\nabla C + C\mathbf{v}$$

- The drift velocity of a positively charged dopant ion is given as  $\mathbf{v} = \mu\mathbf{E}$ . ( $\mu$  is the mobility.) For a negatively charged one,  $\mathbf{v} = -\mu\mathbf{E}$ .

# Alternative form

- Manipulation for combining two terms

- The flux is now given as

$$\mathbf{F}_C = -D\nabla C \pm \mu C \mathbf{E}$$

- Also, with the electrostatic potential,  $\phi(\mathbf{r})$ , it can be written as

$$\mathbf{E} = -\nabla\phi$$

- Moreover, we adopt the Einstein relation,  $D = V_T\mu$ . ( $V_T$  is the thermal voltage.)

- Then,

$$\mathbf{F}_C = -D \left( \nabla C \pm \frac{1}{V_T} C \nabla \phi \right)$$

- It looks good, but how can we calculate  $\phi$ ?

# Approximation for $\phi$

- At equilibrium, (← How can we assume the equilibrium?)

- We can express the electron density,  $n$ , as

$$n = n_{int} \exp \frac{\phi}{V_T}$$

- In other words,  $\phi = V_T \log \frac{n}{n_{int}}$ . Then,

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

- By using the above expression, we have

$$\mathbf{F}_C = -D \left[ \nabla C \pm C \nabla \left( \log \frac{n}{n_{int}} \right) \right]$$

# Approximation for $\phi$

- Finally,

$$\mathbf{F}_C = -DC \left[ \nabla \log C \pm \nabla \left( \log \frac{n}{n_{int}} \right) \right]$$

- Well, instead of  $\phi$ , now we have  $n$ .
- In a rigorous sense, we must calculate  $n$ . (However, it costs.)
- Under the charge neutrality at equilibrium,

$$\begin{aligned} N_D^+ + p &= N_A^- + n \\ np &= n_{int}^2 \end{aligned}$$

- Then, the electron density is obtained as

$$n = \frac{(N_D^+ - N_A^-) + \sqrt{(N_D^+ - N_A^-)^2 + 4n_{int}^2}}{2}$$

# Discretization

- In 1D,

$$F_C = -DC \left[ \frac{\partial}{\partial x} \log C \pm \frac{\partial}{\partial x} \left( \log \frac{n}{n_{int}} \right) \right]$$

- How can we discretize the flux?
- We adopt the “logarithmic flux” approximation.

$$F_{C,i+0.5} = -D \sqrt{C(x_i)C(x_{i+1})} \frac{1}{x_{i+1} - x_i} \left[ \begin{array}{l} \log C(x_{i+1}) \pm \log \frac{n(x_{i+1})}{n_{int}} \\ - \log C(x_i) \mp \log \frac{n(x_i)}{n_{int}} \end{array} \right]$$

- It is nonlinear.

# HW#6

- Due: AM08:00, September 18

- Problem#1

- The intrinsic carrier concentration in silicon is given by

$$n_{int} = 3.1 \times 10^{16} T^{1.5} \exp\left(-\frac{0.603 \text{ eV}}{k_B T}\right) \text{ cm}^{-3}$$

Draw the electron density,  $n$ , as a function of temperature,  $T$ . The temperature varies from 300 K to 1200 K.

Assume the charge neutrality at equilibrium. Consider three values of  $N_D^+ - N_A^-$  :  $10^{20} \text{ cm}^{-3}$ ,  $10^{18} \text{ cm}^{-3}$ , and  $10^{16} \text{ cm}^{-3}$



# Nonlinearity

# Discretized diffusion equation

- It is much more difficult.

- Although it can be generally written as

$$\frac{C(x_i, t_k) - C(x_i, t_{k-1})}{\Delta t} \Delta x = F_{C,i+0.5} - F_{C,i-0.5}$$

- Now, the flux terms are nonlinear,

$$F_{C,i+0.5} = -D \sqrt{C(x_i, t_k) C(x_{i+1}, t_k)} \frac{1}{\Delta x} \left[ \log C(x_{i+1}, t_k) \pm \log \frac{n(x_{i+1}, t_k)}{n_{int}} \right. \\ \left. - \log C(x_i, t_k) \mp \log \frac{n(x_i, t_k)}{n_{int}} \right]$$

- Note that even the electron density is nonlinear.

# Is it $Ax = b$ ?

- Try to construct a matrix,  $A$ , for the flux term.
  - What is the entry for  $C(x_i, t_k)$ ?
- Recall the previous case.
  - In our previous simple problem, the discretized form was

$$\frac{C(x_i, t_k) - C(x_i, t_{k-1})}{\Delta t} \Delta x$$
$$= -D \frac{1}{\Delta x} [C(x_{i+1}, t_k) - C(x_i, t_k)] + D \frac{1}{\Delta x} [C(x_i, t_k) - C(x_{i-1}, t_k)]$$

# Nonlinearity is the key.

- At present, we cannot solve the problem, because it is nonlinear.
  - Let us learn how to solve a nonlinear problem!
- An example, calculation of  $n$  under the charge neutrality.

$$\begin{aligned}N_D^+ + p &= N_A^- + n \\ np &= n_{int}^2\end{aligned}$$

- By eliminating  $p$ , we find an equation of

$$n^2 - (N_D^+ - N_A^-)n - n_{int}^2 = 0$$

- Of course, we know the solution. However, instead of using the known formula, just calculate  $n$  with a numerical method.

# Newton method

- First, we assume an initial solution,  $n_0$ .
  - Of course, there is no guarantee that  $n_0$  is the solution. Therefore,
$$n_0^2 - (N_D^+ - N_A^-)n_0 - n_{int}^2 = r_0 \neq 0$$
  - However, we assert that an improved solution,  $n_1$ , is the real solution. Our assertion can be written as
$$n_1^2 - (N_D^+ - N_A^-)n_1 - n_{int}^2 = 0$$
  - We can take the difference between two equations:
$$(n_1 + n_0)(n_1 - n_0) - (N_D^+ - N_A^-)(n_1 - n_0) = -r_0$$
  - We CANNOT solve, because it is still a nonlinear equation of  $n_1$ .
  - Instead, we can solve the following (approximate) equation:
$$2n_0(n_1 - n_0) - (N_D^+ - N_A^-)(n_1 - n_0) = -r_0$$

# Iteration

- Unfortunately, the solution,  $n_1 - n_0$ , is not exact.
  - Anyway, from  $n_0$  and  $n_1 - n_0$ , we can calculate (inaccurate)  $n_1$ .
  - Then, from  $n_1$ , we again assert that  $n_2$  is the real solution.
  - Again,  $n_2$  will not be perfect.
  - Even though it is not perfect, it may approach to the solution.
  - Repeat this procedure until the error is sufficiently reduced.

# HW#6

- Problem#2

- Calculate the electron density,  $n$ , under the charge neutrality. Adopt the Newton method. Verify your results at two temperatures (300 K and 1200 K) and three dopants densities,  $N_D^+ - N_A^-$  ( $10^{20} \text{ cm}^{-3}$ ,  $10^{18} \text{ cm}^{-3}$ , and  $10^{16} \text{ cm}^{-3}$ ). Of course, your solution should be very close to the analytic solution.

# Thank you!