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 (# cm^{-2} 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
$$\mathbf{E} = -\nabla\phi$$
  - Morever, 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 ϕ?

Approximation for ϕ

- 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 ϕ

- Finally,

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

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

$$N_D^+ + p = N_A^- + n$$
$$np = n_{int}^2$$

  - 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.

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

  - It is nonlinear.

HW#6

- Due: AM08:00, September 18
- Problem#1
  - The intrinsic carrier concentration in silicon is given by

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

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} cm^{-3}, 10^{18} cm^{-3}, and 10^{16} 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,

$$F_{C,i+0.5}$$

$$= -D\sqrt{C(x_i, t_k)C(x_{i+1}, t_k)} \frac{1}{\Delta x} \begin{bmatrix} \log C(x_{i+1}, t_k) \pm \log \frac{n(x_{i+1}, t_k)}{n_{int}} \\ - \log C(x_i, t_k) \mp \log \frac{n(x_i, t_k)}{n_{int}} \end{bmatrix}$$

  - Note that even the electron density is nonlinear.

Is it $\boldsymbol{Ax = b}$?

- 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, calcation of n under the charge neutrality.

$$N_D^+ + p = N_A^- + n$$
$$np = n_{int}^2$$

  - 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 calcultate (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.

Thank you!