Computational Microelectronics
Lecture 5 Diffusion

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Diffusion – Boundary Condition

Zero flux at top surface

- Let us assume the flux at the top surface vanishes.
  - Then, the first row is modified.

$$\frac{1}{t_k - t_{k-1}}\begin{bmatrix} C(x_0, t_k) \\ C(x_1, t_k) \\ \vdots \\ C(x_{N-1}, t_k) \end{bmatrix} - \frac{1}{t_k - t_{k-1}}\begin{bmatrix} C(x_0, t_{k-1}) \\ C(x_1, t_{k-1}) \\ \vdots \\ C(x_{N-1}, t_{k-1}) \end{bmatrix}$$

New boundary condition. *Why?*

$$= \frac{D}{(\Delta x)^2}\begin{bmatrix} -2 & 2 & \cdots & 0 \\ 1 & -2 & 1 & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \cdots & 0 \end{bmatrix}\begin{bmatrix} C(x_0, t_k) \\ C(x_1, t_k) \\ \vdots \\ C(x_{N-1}, t_k) \end{bmatrix}$$

Integrated form

- Original equation

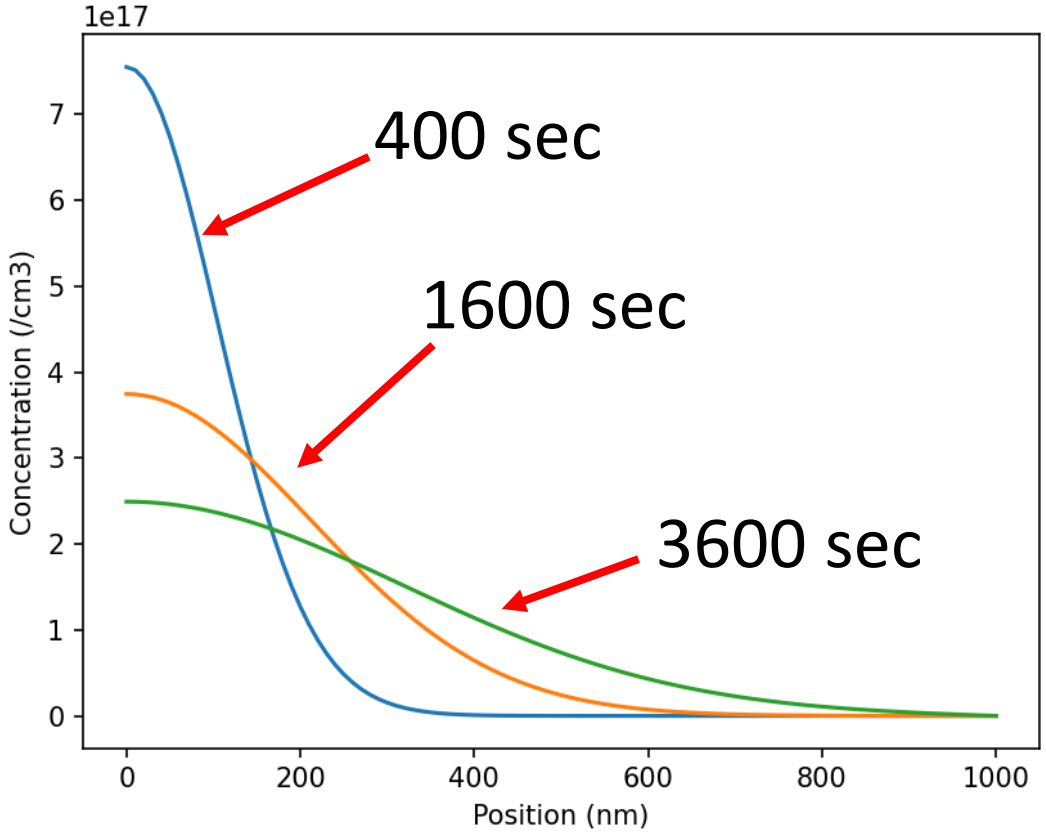
$$\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2}$$

- Integrated equation
  - Integrated over a certain range, $[x_-, x_+]$

$$\frac{\partial}{\partial t}\int_{x_-}^{x_+} C dx = D\left.\frac{\partial C}{\partial x}\right|_{x_+} - D\left.\frac{\partial C}{\partial x}\right|_{x_-}$$

Simulation results

- A similar problem for a half domain
  - Initially, a Dirac-delta-like boron profile with a dose of 1 X 10^{13} cm^{-2}
  - Thermal diffusion for 60 min at 1100 °C (D is 1.42 X 10^{-13} cm^2 sec^{-1}.)



HW#5

- Due: AM08:00, September 13
- Problem#1
  - Reproduce the graph in the last slide.

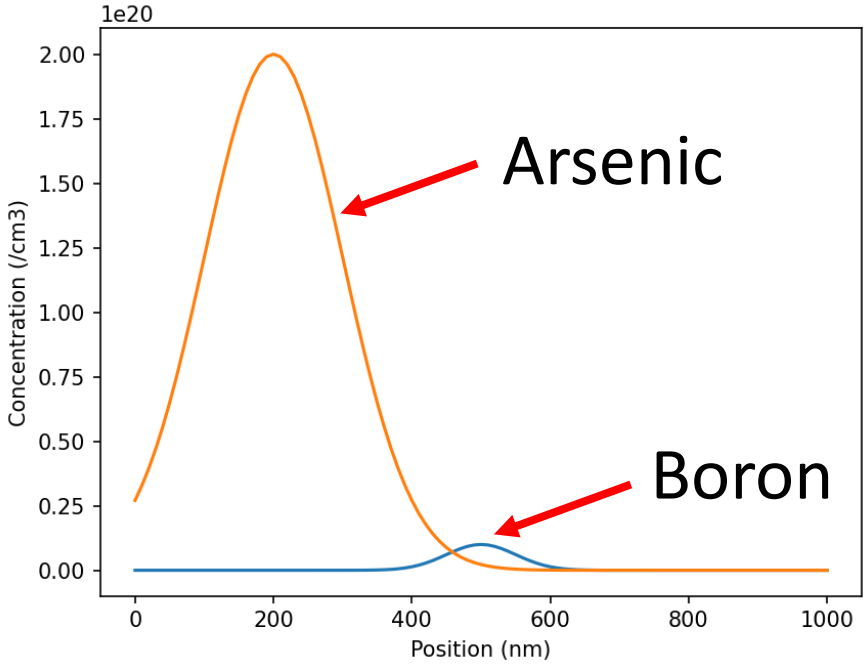
Diffusion – Multiple Species

Multiple dopants

- For example, boron and arsenic
  - We may have two approaches.
  - 1) Calculate each of them, individually.
  - 2) Calculate both of them, simultaneously.
  - In the second approach, the solution vector becomes twice larger.
- Arranging the unknown variables
  - One possible implementation
    $$[C_B(x_0)C_{As}(x_0)C_B(x_1)C_{As}(x_1) \dots C_B(x_{N-1})C_{As}(x_{N-1})]^T$$
  - Another possible implementation
    $$[C_B(x_0)C_B(x_1) \dots C_B(x_{N-1})C_{As}(x_0)C_{As}(x_1) \dots C_{As}(x_{N-1})]^T$$

Example) Boron & arsenic

- Initially, Gaussian profiles. Simulate 60-min-long anneal.
  - B: Peak at 0.5 µm. Peak density is 1.0 X 10^{19} cm^{-3}. Standard deviation is 50 nm. Diffusivity of 1.40 X 10^{-14} cm^2 sec^{-1}
  - As: Peak at 0.2 µm. Peak density is 2.0 X 10^{20} cm^{-3}. Standard deviation is 100 nm. Diffusivity of 1.43 X 10^{-15} cm^2 sec^{-1}



HW#5

- Problem#2
  - Draw the final dopant profiles in the linear-linear scale.
  - Draw the same dopant profiles in the semi-logarithmic scale.

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,

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

Thank you!