Computational Microelectronics L15

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Diffusion

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

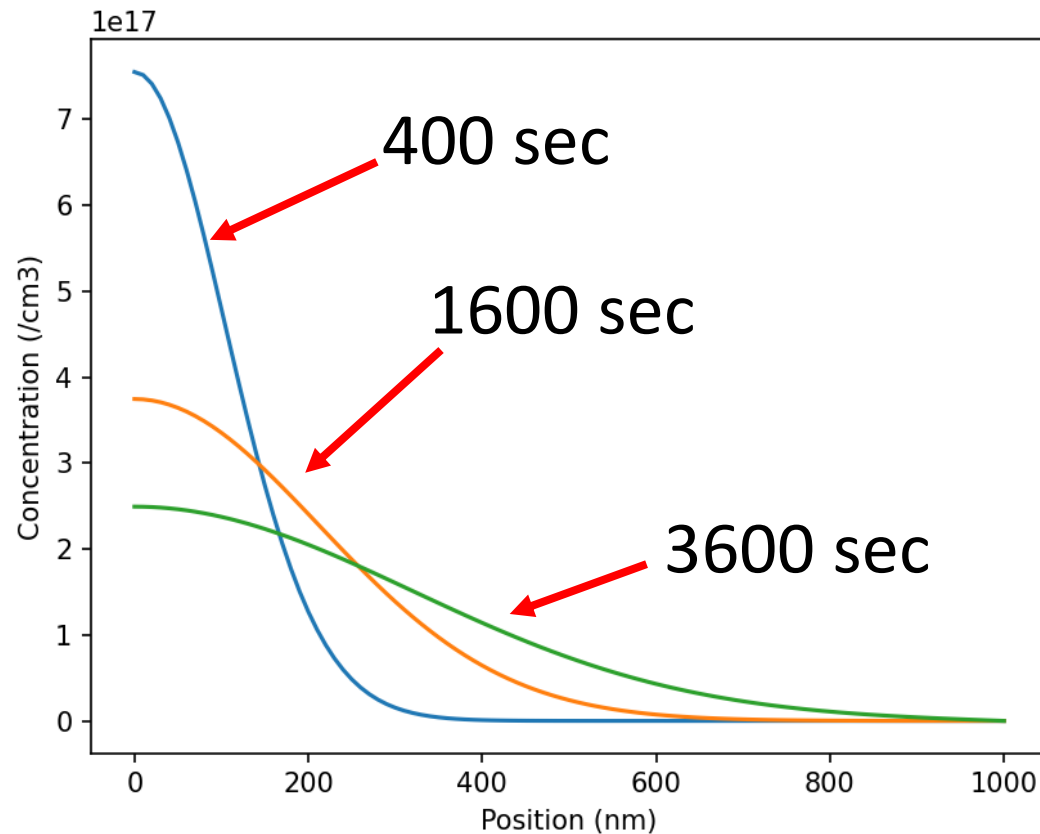$$\frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2}$$

- 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 1×10^{13} cm^{-2}
  - Thermal diffusion for 60 min at 1100 °C (D is 1.42×10^{-13} cm^2 sec^{-1}.)

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
  $$[C_B(x_0)C_{As}(x_0)C_B(x_1)C_{As}(x_1) \ldots C_B(x_{N-1})C_{As}(x_{N-1})]^T$$
  - Another possible implementation
  $$[C_B(x_0)C_B(x_1) \ldots C_B(x_{N-1})C_{As}(x_0)C_{As}(x_1) \ldots C_{As}(x_{N-1})]^T$$

Example

- Consider the following initial profiles and conditions.
  - B: Uniform distribution with a density of 10^{17} cm^{-3}. Diffusivity of 1.40×10^{-14} cm^2 sec^{-1}
  - As: Gaussian profile. Peak at 20 nm. Peak density is 5.0×10^{21} cm^{-3}. Standard deviation is 9 nm. Diffusivity of 1.47×10^{-15} cm^2 sec^{-1}
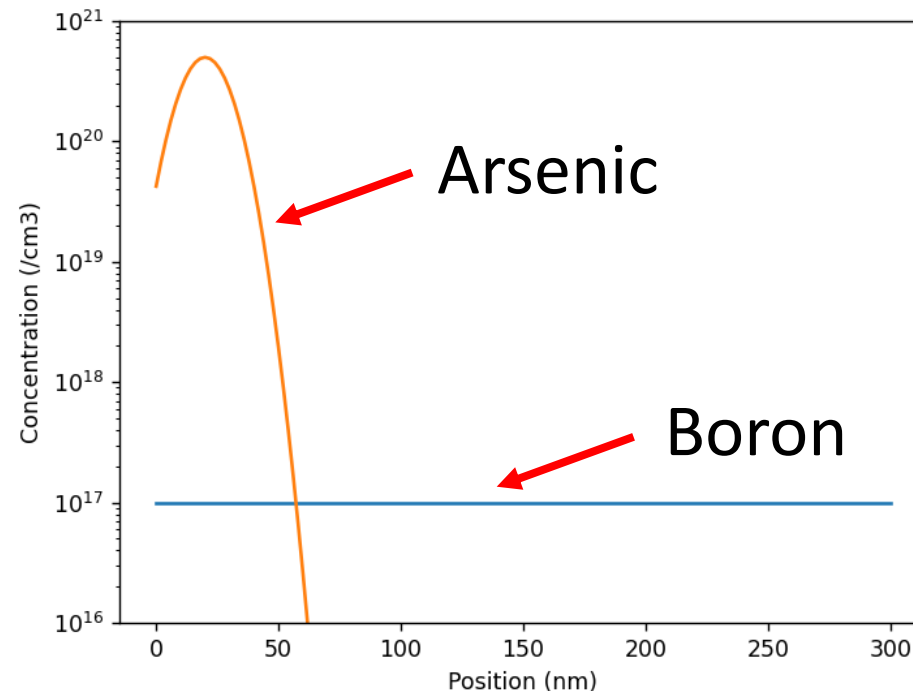
After 10 min. w/o electric field effect

- Without the electric field effect,
  - Boron is still uniformly distributed.
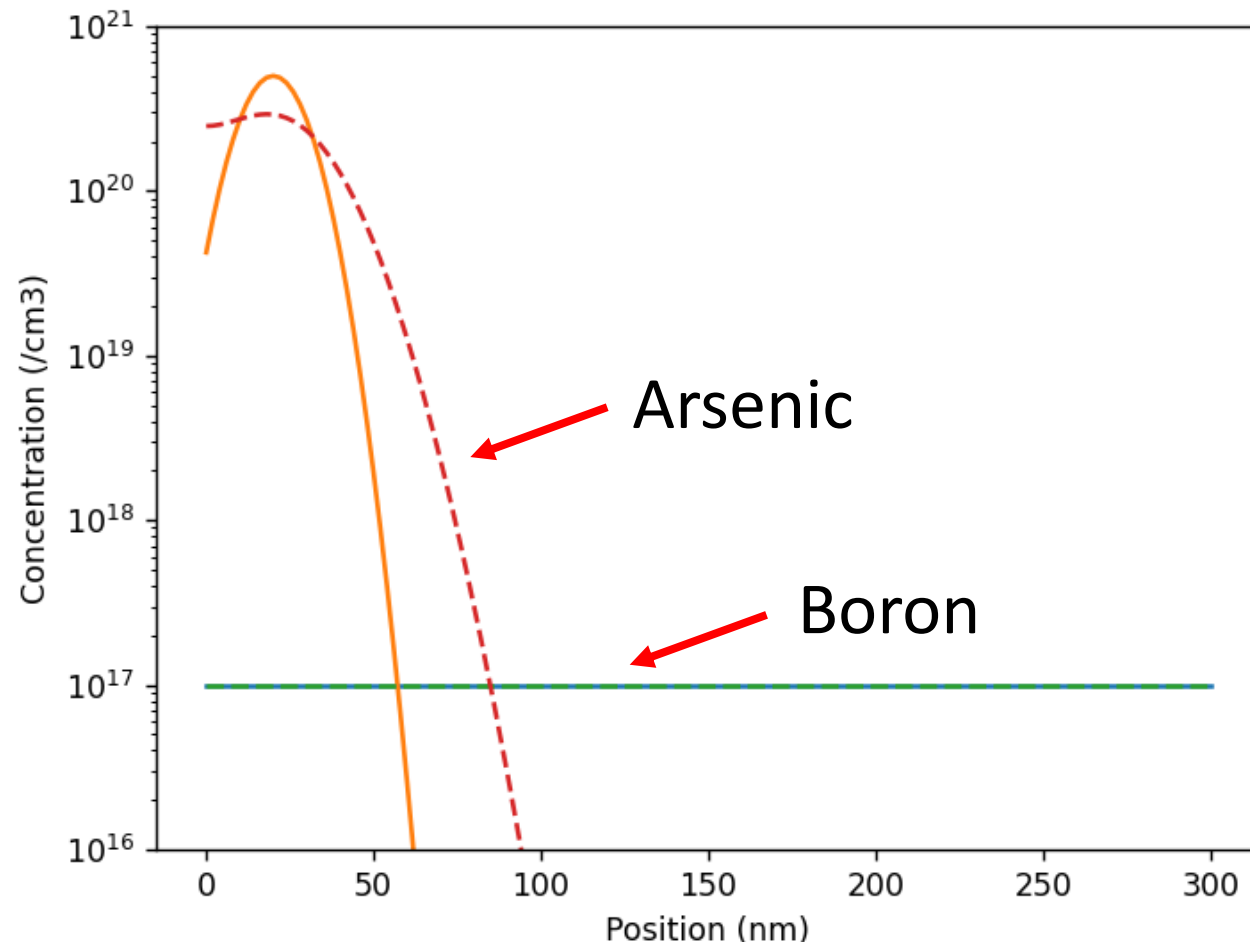
Drift

- 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, $\mathbf{v} = -\mu\mathbf{E}$.

Flux in terms of ϕ

- 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, ($\Leftarrow$ How can we assume the equilibrium?)
  - We can express the electron density, n, as $n = n_{int} \exp \dfrac{\phi}{V_T}$.
  - In other words, $\phi = V_T \log \dfrac{n}{n_{int}}$. Then, $\nabla \phi = V_T \nabla \left(\log \dfrac{n}{n_{int}} \right)$
  - By using the above expression, we have $\mathbf{F}_C = -D \left[\nabla C \pm C \nabla \left(\log \dfrac{n}{n_{int}} \right) \right]$.
  - Under the charge neutrality at equilibrium, $N_D^+ + p = N_A^- + n$ and $np = n_{int}^2$.
  - Then, the electron density is obtained as
  $$n = \frac{(N_D^+ - N_A^-) + \sqrt{(N_D^+ - N_A^-)^2 + 4n_{int}^2}}{2}$$

Nonlinear Poisson equation

- Charge neutrality

- Instead, we can solve the nonlinear Poisson equation
  - At each time instance, using the dopant distribution, calculate the electrostatic potential. (Which is an appropriate boundary condition?)
  - From the calculated ϕ, we can consider the electric field effect. (How can you discretize it?)

Homework#15

- Due: AM08:00, November 12

- Problem#1
  - Consider the electric field effect in the last example. Draw the dopant profiles after 10 minutes. In your calculation, the electrostatic potential should be calculated by solving the nonlinear Poisson equation.
  - Assume that the temperature is 1000 ℃ and the intrinsic carrier density is 7.12×10^{18} cm^{-3}.

Thank you for your attention!