Computational Microelectronics L14

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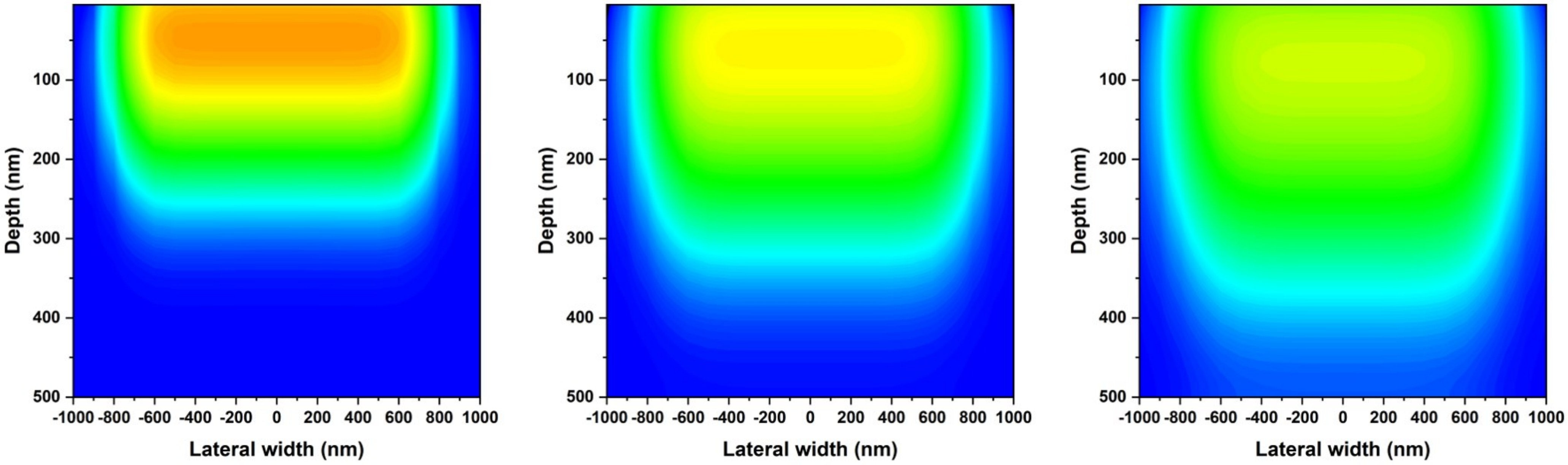
Diffusion

Diffusion process

- Two-step process for producing a junction at the desired depth
  - The predeposition step introduces a controlled number of impurity atoms.
  - The drive-in step thermally diffuses the dopant to the desired junction depth.



Longer diffusion time

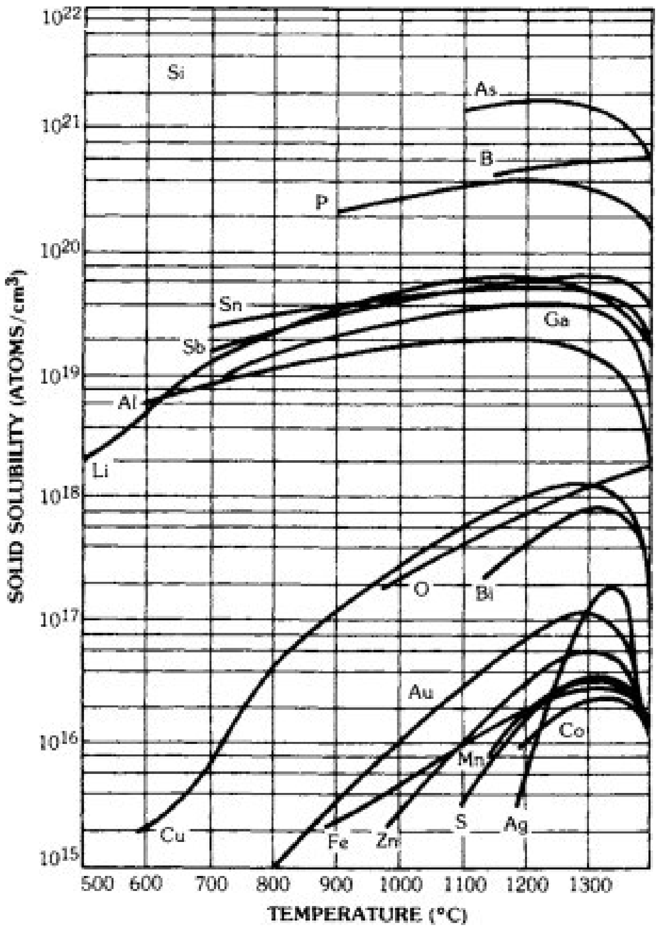
Dopant solid solubility

- The maximum concentration of a dopant that can be dissolved in silicon under equilibrium conditions, without forming a separate phase
  - The electrical solubility limt may be lower.
  - Example) Arsenic

  Its maximum solid solubility is about $2X10^{21}$ cm^{-3}.

  (Maximum) active arsenic concentration

  is about $2X10^{20}$ cm^{-3}.



Solid solubility curves for various dopants in silicon (Trumbore, Bell System Technical Journal, 1960.)

Macroscopic/microscopic viewpoints

- Macroscopic viewpoint
  - Considering the dopant profile, $C(\mathbf{r})$
  - Predicting the time evolution of $C(\mathbf{r})$ by solving a diffusion equation subject to some boundary conditions
- Microscopic viewpoint
  - Atomistic scale
  - Trying to relate the overall motion of the whole profile to the individual motions of unseen atoms based on interactions of atoms and point defects in the lattice

Macroscopic diffusion equation

- Continuity of dopant atoms

$$\frac{\partial C}{\partial t} = -\nabla \cdot \mathbf{F}_C$$

  - What is $\mathbf{F}_C$? The flux is written as (# cm^{-2} sec^{-1})

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

  - Here, D is the diffusivity. (cm^{2} sec^{-1})
  - When two equations are combined, we have

$$\frac{\partial C}{\partial t} = \nabla \cdot (D\nabla C)$$

  - Of course, in 1D and for a constant D, it is simplified as $\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2}$.

Steady-state condition

- At the steady-state, $\frac{\partial C}{\partial t}$ vanishes.
  - Therefore, we have a quite simple equation of
$$D\frac{\partial^2 C}{\partial x^2} = 0$$
  - Its solution has the form of
$$C(x) = a + bx$$
  - With two boundary values, $C(x = 0)$ and $C(x = L)$, we can easily calculate a and b.
  - When we know a and b, the solution, $C(x)$, satisfies the diffusion equation everywhere.

Discretization

- Assume the simulation domain of $[0, L]$.
  - We introduce a finite number of points,
  $$x_0 (\equiv 0), x_1, \dots, x_{N-1} (\equiv L)$$
  - For a uniform grid,
  $$x_i = i \times \frac{L}{N-1} = i \times \Delta x$$
  - Also, we introduce the dopant concentrations at those points,
  $$C(x_0), C(x_1), \dots, C(x_{N-1})$$
  - Instead of finding out $C(x)$, which satisfies the diffusion equation everywhere, we try to find a solution vector, $[C(x_0)\ C(x_1)\ \dots\ C(x_{N-1})]^T$, which satisfies the diffusion equation (or the boundary conditions) at those discretized points only.

Example) $N = 6$

- For this specific number,
  - We construct the following system of equations:

$$\begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ & & \text{Discretized equation at } x_1 & & & \\ & & \text{Discretized equation at } x_2 & & & \\ & & \text{Discretized equation at } x_3 & & & \\ & & \text{Discretized equation at } x_4 & & & \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} C(x_0) \\ C(x_1) \\ C(x_2) \\ C(x_3) \\ C(x_4) \\ C(x_5) \end{bmatrix} = \begin{bmatrix} C(0) \\ 0 \\ 0 \\ 0 \\ 0 \\ C(L) \end{bmatrix}$$

  - How can we discretize the equation?

Discretization of second-order derivative

- Assume a uniform grid.
  - At x_i, the second derivative term is approximated as

$$\frac{\partial^2 C}{\partial x^2} \approx \frac{C(x_{i+1}) - 2C(x_i) + C(x_{i-1})}{(\Delta x)^2}$$

  - Then, the discretized equation at x_i can be written as

$$D\,\frac{C(x_{i+1}) - 2C(x_i) + C(x_{i-1})}{(\Delta x)^2} = 0$$

  - Multiplying $\frac{(\Delta x)^2}{D}$, we have

$$C(x_{i+1}) - 2C(x_i) + C(x_{i-1}) = 0$$

Discretized equation at x_i

Diffusion equation with $N = 6$

- Using the previous form,
  - We explicitly construct the resultant system as

$$\underbrace{\begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & -2 & 1 & 0 & 0 & 0 \\ 0 & 1 & -2 & 1 & 0 & 0 \\ 0 & 0 & 1 & -2 & 1 & 0 \\ 0 & 0 & 0 & 1 & -2 & 1 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}}_{\mathbf{A}} \underbrace{\begin{bmatrix} C(x_0) \\ C(x_1) \\ C(x_2) \\ C(x_3) \\ C(x_4) \\ C(x_5) \end{bmatrix}}_{\mathbf{x}} = \underbrace{\begin{bmatrix} C(0) \\ 0 \\ 0 \\ 0 \\ 0 \\ C(L) \end{bmatrix}}_{\mathbf{b}}$$

Diffusion equation in 1D

- In general, $\frac{\partial C}{\partial t}$ does not vanish.
  - Therefore, we must solve the following equation:

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

  - In the previous lecture, $\frac{\partial^2 C}{\partial x^2}$ was discretized.

$$\frac{\partial^2 C}{\partial x^2} \approx \frac{C(x_{i+1}) - 2C(x_i) + C(x_{i-1})}{(\Delta x)^2}$$

  - The remaining task is to discretize $\frac{\partial C}{\partial t}$.

In a vector form

- Solution vector, $[C(x_0)\ C(x_1)\ \ \ldots\ \ C(x_{N-1})]^T$
  - Then, in the backward Euler scheme, the time derivative can be written as

$$\left.\frac{\partial C}{\partial t}\right|_{t_k} \rightarrow \frac{1}{t_k - t_{k-1}} \begin{bmatrix} C(x_0, t_k) \\ C(x_1, t_k) \\ \vdots \\ C(x_{N-1}, t_k) \end{bmatrix} - \frac{1}{t_k - t_{k-1}} \begin{bmatrix} C(x_0, t_{k-1}) \\ C(x_1, t_{k-1}) \\ \vdots \\ C(x_{N-1}, t_{k-1}) \end{bmatrix}$$

Discretized diffusion equation

- Let us assume the fixed C values at two boundaries.
  - Then, in the backward Euler scheme,

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

Boundary condition

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

Boundary condition

Unknown and known variables

- $C(x_i, t_k)$ is unknown, while $C(x_i, t_{k-1})$ is known.
  - After simple manipulation,

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

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

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It is $\mathbf{Ax} = \mathbf{b}$, again.

- In this form,

$$\mathbf{A} = \frac{1}{t_k - t_{k-1}}\begin{bmatrix} 1 & 0 & \cdots & 0 \\ 0 & 1 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \cdots & 1 \end{bmatrix} - \frac{D}{(\Delta x)^2}\begin{bmatrix} 0 & 0 & \cdots & 0 \\ 1 & -2 & 1 & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \cdots & 0 \end{bmatrix}$$

$$\mathbf{x} = \begin{bmatrix} C(x_0, t_k) \\ C(x_1, t_k) \\ \vdots \\ C(x_{N-1}, t_k) \end{bmatrix} \text{ and } \mathbf{b} = \frac{1}{t_k - t_{k-1}}\begin{bmatrix} C(x_0, t_{k-1}) \\ C(x_1, t_{k-1}) \\ \vdots \\ C(x_{N-1}, t_{k-1}) \end{bmatrix}$$

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Implementation

- Start from the initial dopant profile.
  - Calculate a new dopant profile by solving the discretized diffusion equation.
  - Repeat this process until the time reaches at its target value.

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Example) Boron diffusion

- Initially, a Dirac-delta-like profile with a dose of 2 X 10^{13} cm^{-2}
  - Thermal diffusion for 60 min at 1100 °C
  - Diffusivity follows

$$D = D^0 \exp\left(-\frac{E_A}{k_B T}\right)$$

  - For borons, D^0 is 1.0 cm^2 sec^{-1} and E_A is 3.5 eV.
  - Then, at 1100 °C, D is about 1.42 X 10^{-13} cm^2 sec^{-1}.

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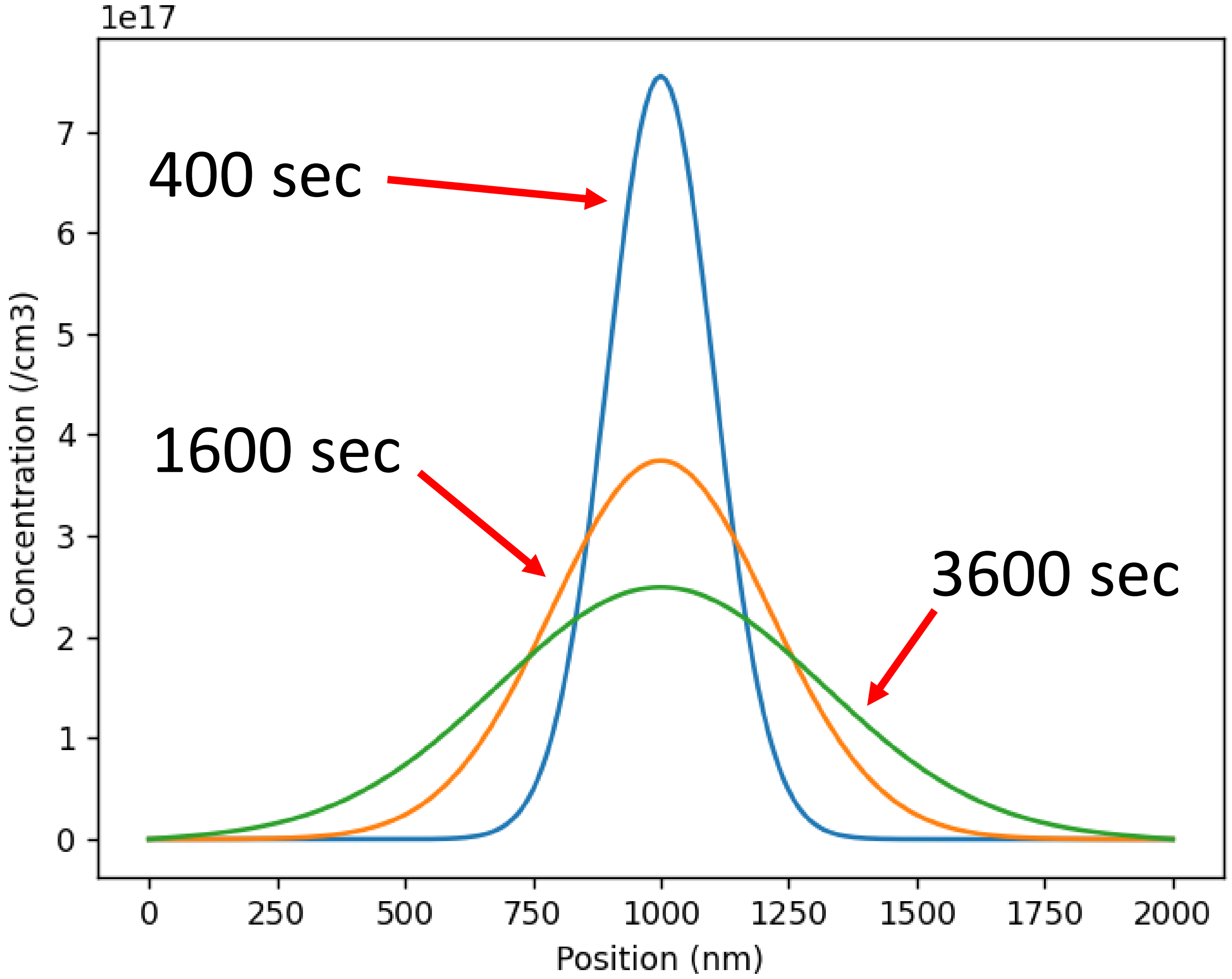
Simulation parameters

- Real space
  - 1001 mesh points with 10 nm spacing
  - Initially, at 500th point, 2 X 10^{19} cm^{-3}. (Match the dose.) At all other points, the concentration vanishes.
- Time
  - Time evolves from 0 to 3600 sec.

Simulation results

- Dopant profiles at some time instances (400 sec, 1600 sec, and 3600 sec)
  - Gaussian profile
  - Peak ~ $\frac{1}{\sqrt{Dt}}$



Homework#14

- Due: AM08:00, November 7
- Problem#1
  - Implement the diffusion solver. Verify your simulation results against the graph shown in this lecture. Also, test the same problem at 1000 °C. (Since the temperature is lower, the diffusion becomes quite weak. Modify your simulation parameters for this lower temperature.)

Thank you for your attention!