# Computational Microelectronics
# Lecture 3 Diffusion

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# Matrix solver

# Matrix solver for $Ax = b$

- In this course, we must solve the matrix equation, $Ax = b$.
  - $A$: A square matrix, whose size is $N \times N$
  - $b$: A vector, whose size is $N \times 1$
  - $x$: A solution vector, whose size is $N \times 1$
  - We assume that $A$ and $b$ are known. Caluculate $x$.
- How to solve $Ax = b$ in various environments
  - MATLAB: It provides `x = A \ b`
  - Python: It provides `x = np.linalg.solve(A, b)`
  - C++: LAPACK

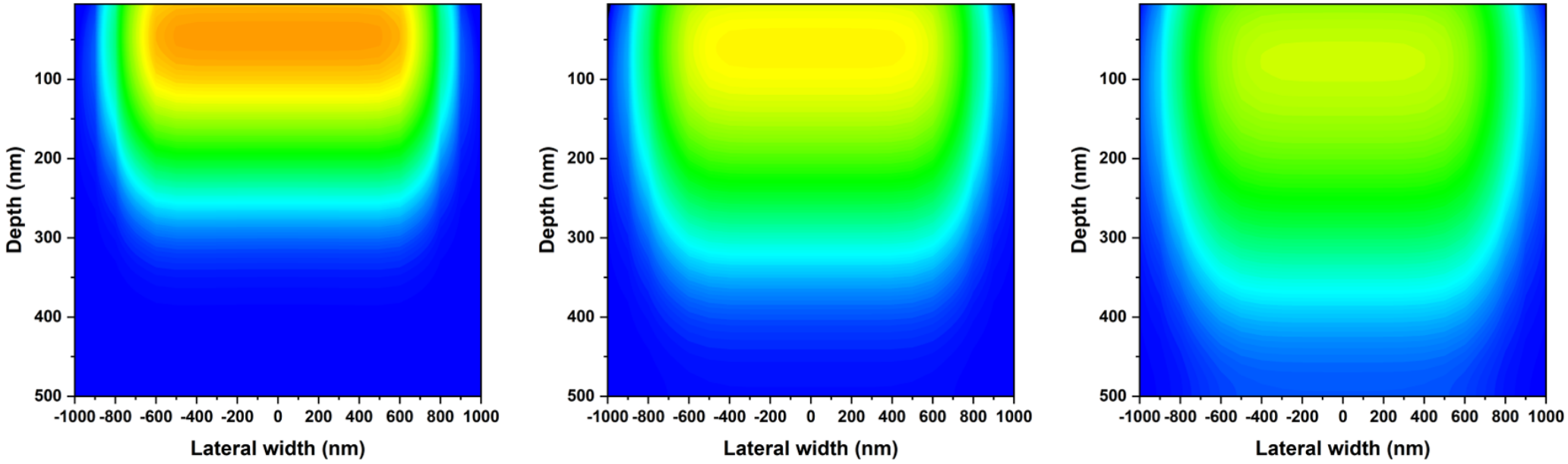
# HW#3

- Due: AM08:00, September 6
- Problem#1
  - A user provides six double-precision numbers in a text file. Load the text file and construct $Ax = b$. For example, the first four entries can be used for the 2X2 matrix, $A$, and the last two for the 2X1 vector, $b$. Then, calculate the solution vector, $x$. Verify your code with various examples.

# 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.



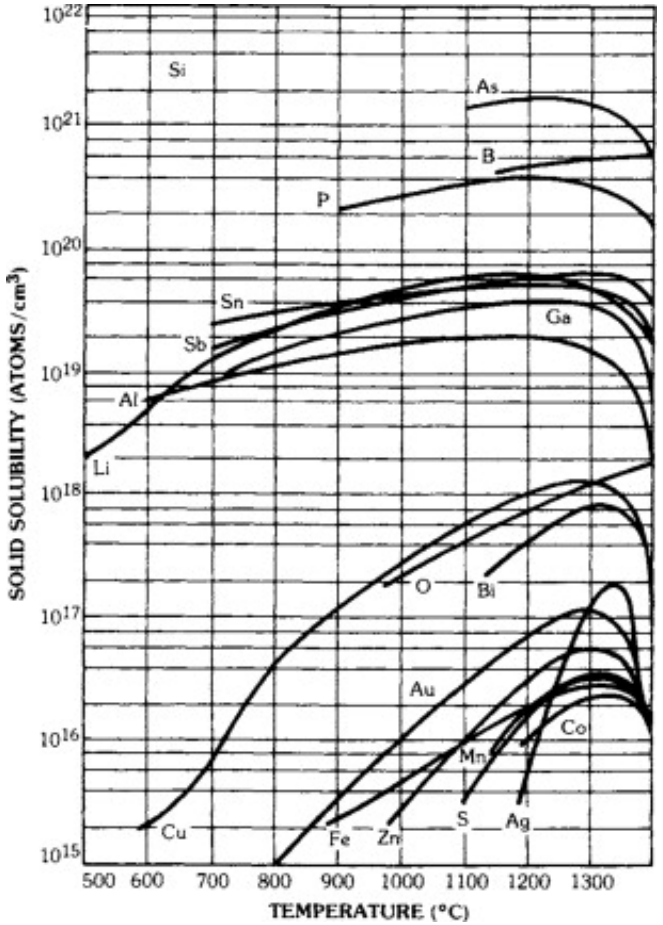

Longer diffusion time

# 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 and 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,
    $$x_0(\equiv 0), x_1, \ldots, x_{N-1}(\equiv L)$$
  - 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,
    $$C(x_0), C(x_1), \ldots, C(x_{N-1})$$
  - Instead of finding out $C(x)$, which satisfies the diffusion equation everywhere, we try to find a solution vector, $[C(x_0)\ C(x_1)\ \ldots\ C(x_{N-1})]^T$, 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

$$\begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & -2 & 1 & 0 & 0 & 0 \\ 0 & 1 & -2 & 1 & 0 & 0 \\ 0 & 0 & 1 & -2 & 1 & 0 \\ 0 & 0 & 0 & 1 & -2 & 1 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} C(x_0) \\ C(x_1) \\ C(x_2) \\ C(x_3) \\ C(x_4) \\ C(x_5) \end{bmatrix} = \begin{bmatrix} C(0) \\ 0 \\ 0 \\ 0 \\ 0 \\ C(L) \end{bmatrix}$$

$A$ $x$ $b$

# HW#3

- Problem#2
  - Consider a 100-nm-long structure. The donor concentration at one end is $10^{20}$ $cm^{-3}$, while it is $10^{17}$ $cm^{-3}$ at the other end. Solve the steady-state diffusion equation numerically, with 6 uniform grid points. Compare your numerical solution with the analytic solution.

# Thank you!