

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. Calculate x .
 - How to solve $Ax = b$ in various environments
 - MATLAB: It provides $x = A \setminus b$
 - Python: It provides $x = \text{np.linalg.solve}(A, b)$
 - C++: LAPACK
- Numpy is needed. 

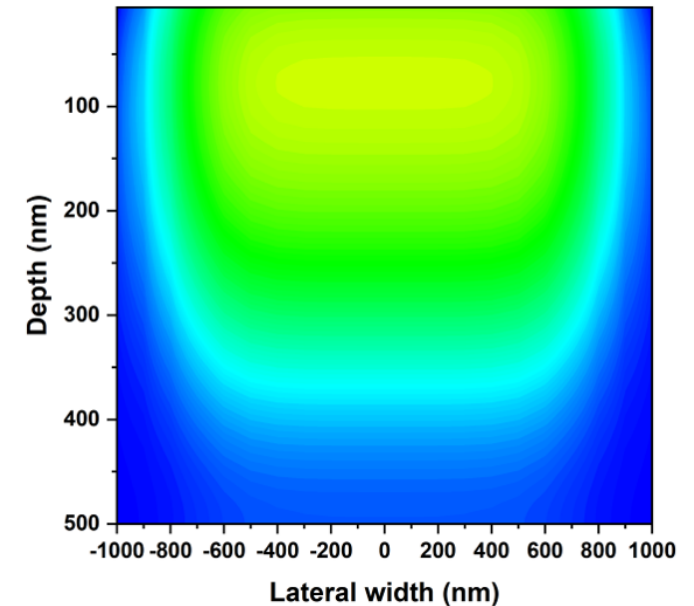
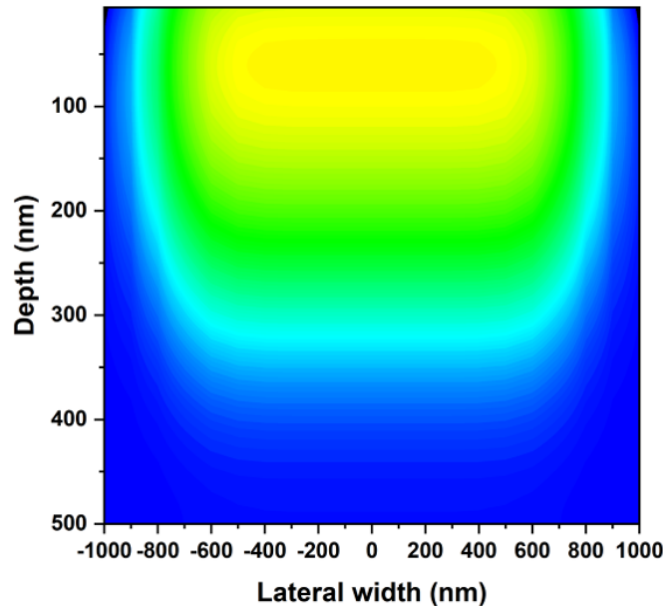
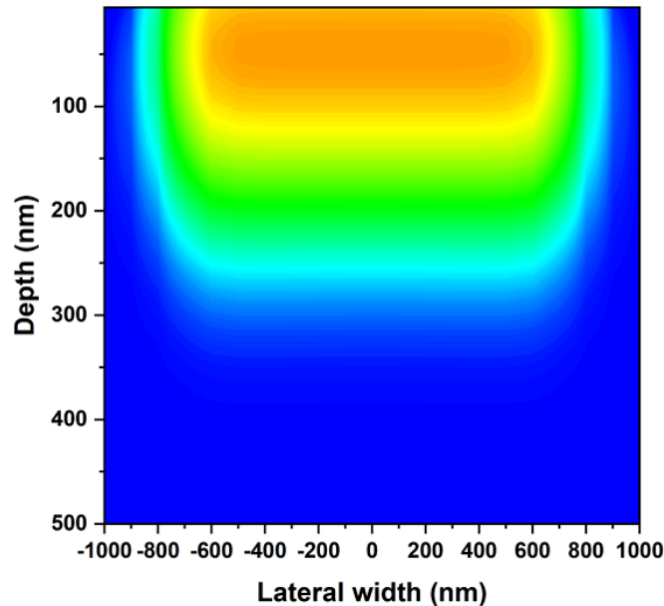
HW#3

- 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 limit may be lower.

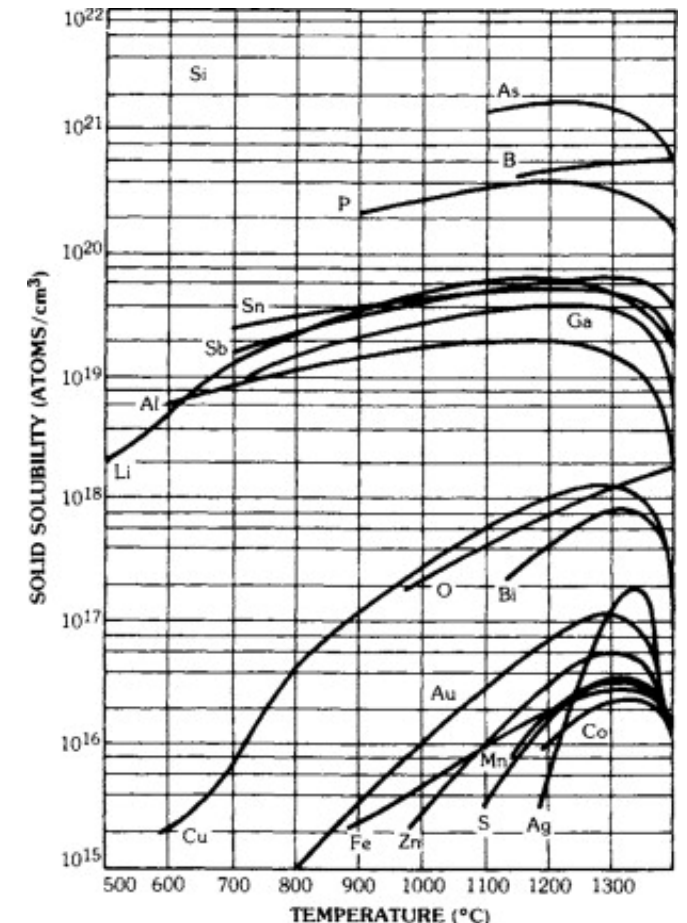
- Example) Arsenic

Its maximum solid solubility is about $2 \times 10^{21} \text{ cm}^{-3}$.

(Maximum) active arsenic concentration

is about $2 \times 10^{20} \text{ cm}^{-3}$.

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 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 ($\# \text{ cm}^{-2} \text{ sec}^{-1}$)

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

- Here, D is the diffusivity. ($\text{cm}^2 \text{ sec}^{-1}$)
- 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

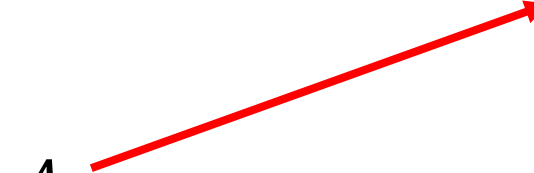
$$C(x_{i+1}) - 2C(x_i) + C(x_{i-1})) = 0$$

Discretized equation at x_i


Diffusion equation with $N = 6$

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


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



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!