Due date – 8th Sep 2023

EE 735 MSL

Assignment-4

Diffusion

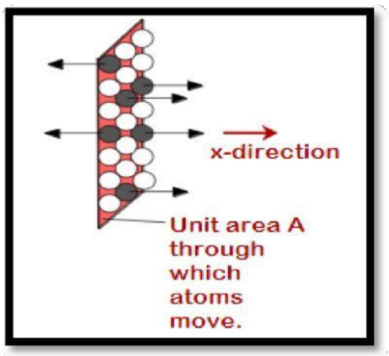
What is diffusion?

- It is defined as **movement of particle from a region of higher conc.to a region of lower conc**.
- Diffusion is driven by concentration gradient
- Observed everywhere from atoms (in doping), ele ctrons and holes(diffusion current) to ions in bio-molecular processes.

Flux:

- The flux of diffusing particles J is used to quantify how fast the process is.
- It is defined **as no of particles diffusing per unit cross-sectionalarea per unit time**.

$$J=(1/A)\ dN/dt$$



Fick’s First Law (steady-state diffusion):

- The diffusion along a fixed direction is proportional to the concentration gradient. $\boxed{J = -D * \{dC/dX\}}$

Above equation is called **Fick’s 1st law**.

{Equation 7.6 in VLSI Technology by Plummer}

Where, D is the diffusion coefficient called Diffusivity. It is a material property.

- The **minus** sign indicates that the diffusion is in the direction of decreasing concentration.

Fick’s Second Law (Non-steady state diffusion):

- If a flux of particles in entering **at x** at **time t** and leaving at **x+Δx** at **time t+Δt**
- The concentration change dC= (J(x+Δx)-J(x))dtA /Adx

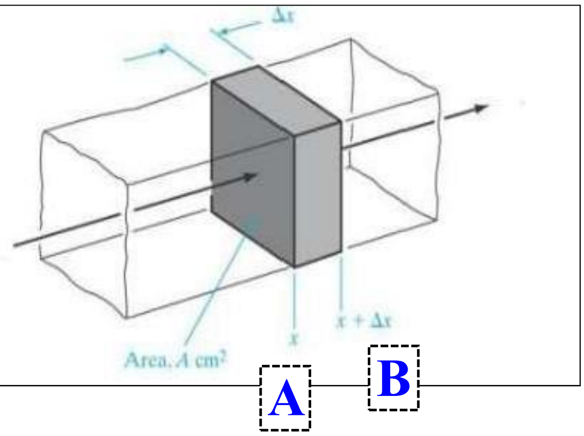
{Fick’s 2nd law, ref -7 (VLSI Tech by Plummer)}

This reduces to:

$$\frac{\partial C}{\partial t} = -\frac{\partial J}{\partial x}$$

From 1st law, putting value of J, we get

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



The diffusion equation:

- The diffusion equation is

$$\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2} \qquad \nabla^2 C = \frac{1}{D}\frac{\partial C}{\partial t} \quad \text{(3-D)}$$

where D is diffusivity.

- If the concentration (**C**) is **time-independent** the equation reduces to {as, dC/dt =0}

$$\nabla^2 C = 0$$

Solving the equation numerically:

- The diffusion equation $\frac{d^2 n}{dx^2} - \frac{1}{D}\frac{dn}{dt} = 0$

$$\left(\frac{d^2}{dx^2} - \frac{1}{D}\frac{d}{dt}\right) n = 0$$

- Any differential equation of the type

Of(x)=g(x)

where O is the differential operator **f(x)** is the **response** and **g(x)** is the **source** .

- Also, If g(x)=0, the equation is homogeneous.
- There can be various sources of non-homogeneity

Using
Central
Diff.
Formula

- The equation can be written numerically

$$\frac{d^2 n}{dx^2} = \frac{n_{i+1,m} - 2n_{i,m} + n_{i-1,m}}{h^2} \qquad \frac{dn}{dt} = \frac{n_{i,m} - n_{i,m-1}}{p}$$

Using
Backword
Diff.
Formula

- So diffusion equation becomes {After substituting above eqns}

$$\frac{n_{i+1,m} - 2n_{i,m} + n_{i-1,m}}{h^2} - \frac{n_{i,m} - n_{i,m-1}}{Dp} = 0$$

- Where **i** and **m** are indices in **position** domain and **time** domain.
- For some source the equation will become

$$\frac{n_{i+1,m} - 2n_{i,m} + n_{i-1,m}}{h^2} - \frac{n_{i,m} - n_{i,m-1}}{Dp} = S$$

EE 735

Assignment-4

Diffusion

(Part-A)

Due date – 8th Sep 2023

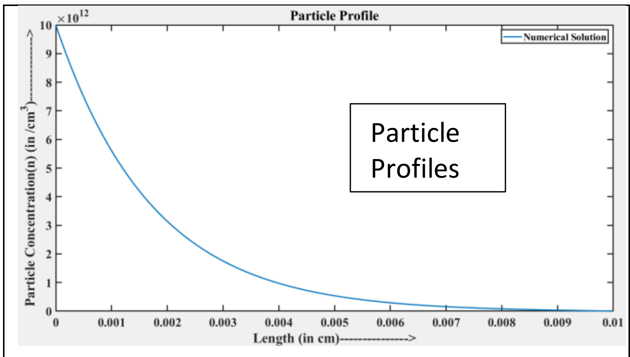
Problem 1: Consider a region of length 10μm from point A (x= 0μm) to point B (x= 10μm).

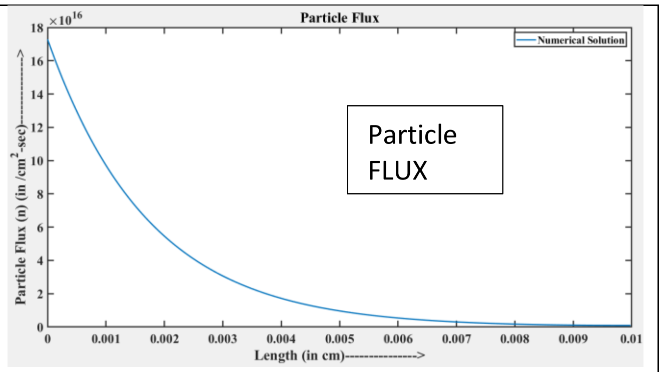
a) Time-Independent Part:

$$D\frac{d^2n}{dx^2} = \frac{n}{\tau}$$

Consider diffusive transport of particles from point A to point B. The **concentration of particles at A is n=10^{12}** cm^{-3}, and at B is n=0 cm^{-3}. Assume τ=10^{-7} s. Find the particle profile from A to B. What is the particle flux from A to B?

In continuation, assume that the **boundary condition at B** is such that $J = kn$, where J is the particle flux (outgoing), $k = 10^3\ cm/s$, and n is the particle density. Again, find the particle profile from A to B and the particle flux at B. Explore the implications of this change in boundary conditions at B.





Note: Only Steady state Continuity equations
Without time dependence.

Now consider the injection of particle flux/density in between point A to B.

b) In Continuation:

Assume that **particle flux** is introduced midway at **x= (3 +0.5 * X)μm** {where, X= last digit of Roll No. from 0 to 9}at the **rate of 10^{13} cm^{-2} /s.** Assume that the particle densities at points A and B are held constant at **n=0.** Assume τ = **10^{-7} s**. Find the **particle profile** from A to B, and the flux at A and B. Also, compare with the analytical resulting the same plot **(use D = 0.1cm^{-2}/s).**

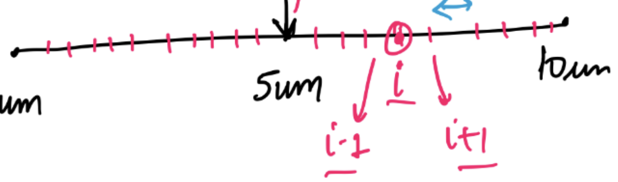
$$D\frac{d^2n}{dx^2} = \frac{n}{\tau}$$

Numerical Solution of Steady State Equation: →

$$\boxed{D\frac{d^2n}{dx^2} = \frac{n}{\tau}}$$

Diffusive Transport

$\Delta x \rightarrow$ distance b/w 2 steps taken



from Central difference formula:- we can write this equation numerically as.

$$D * \left\{\frac{n(i-1) - 2n(i) + n(i+1)}{\Delta x^2}\right\} = \frac{n(i)}{\tau} \quad \text{for } i\text{th Node}$$

Rearranging above equation

$$\left(\frac{1}{\Delta x^2}\right) n_{i-1} + \left(-\frac{2}{\Delta x^2} - \frac{1}{D\tau}\right) n_i + \left(\frac{1}{\Delta x^2}\right) n_{i+1} = 0 \quad \left\{\begin{array}{c}\text{For } 2^{nd} \text{ to} \\ (n-1)^{th} \text{ Node}\end{array}\right\}$$

In Matrix form,

1st BC

Middle B.C

Last Node BC

$$\begin{bmatrix} \frac{1}{\Delta x^2} & -\left(\frac{2}{\Delta x^2}+\frac{1}{D\tau}\right) & \frac{1}{\Delta x^2} & 0 & 0 & 0 & 0 & \cdots \\ 0 & \frac{1}{\Delta x^2} & -\left(\frac{2}{\Delta x^2}+\frac{1}{D\tau}\right) & \frac{1}{\Delta x^2} & 0 & 0 & 0 & \cdots \\ & & & \vdots & & & & \\ \cdots & 0 & 0 & \frac{1}{\Delta x^2} & -\left(\frac{2}{\Delta x^2}+\frac{1}{D\tau}\right) & \frac{1}{\Delta x^2} & 0 \\ \cdots & 0 & 0 & 0 & \frac{1}{\Delta x^2} & -\left(\frac{2}{\Delta x^2}+\frac{1}{D\tau}\right) & \frac{1}{\Delta x^2} \end{bmatrix} \begin{bmatrix} n_A \\ n_{A+\Delta x} \\ n_{A+2\Delta x} \\ \vdots \\ n_{i-1} \\ n_i \\ n_{i+1} \\ \vdots \\ n_B \end{bmatrix} = \begin{bmatrix} BC\ 1st \\ 0 \\ 0 \\ 0 \\ \vdots \\ \text{Middle BC} \\ \vdots \\ 0 \\ \text{Last BC} \end{bmatrix}$$

$n \times n$ $n \times 1$ $n \times 1$

Tri-digonal Matrix.

$$A * n = B$$

$$\# \quad \boxed{n = A^{-1} * B}$$

Here, @ $x = 5\mu m$ $J = 10^{13}\ cm^{-2}/sec$ given

This equation @ $x=5$ will corresponds to a particular node in the matrix. Right ??

How to incorporate that B.C:-

$$J = -D\frac{dn}{dx} = 10^{13}$$ {from fick's first law}

from Backward differe formula,

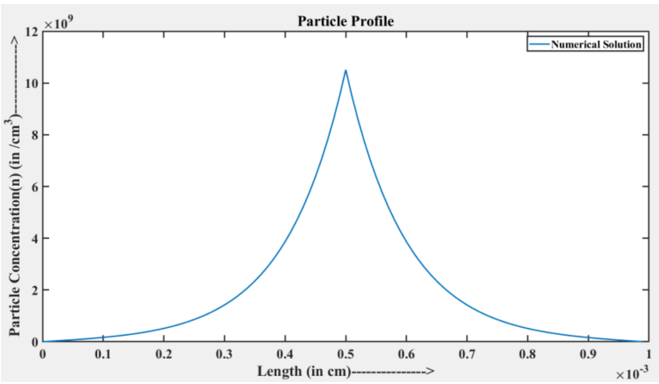
$$\frac{dn}{dx} = \boxed{\frac{n_i - n_{i-1}}{\Delta x} = \frac{10^{13}}{D}}$$

Rearrange this Equation and put in the above matrix @ (5um)

i.e at Correspondy Nodes.

For Analytical solution,

1) Solve the differential equations using basic knowledge
2) Put boundary conditions
3) Match the simulations results with Analytical ones onsame plot. You are good to go.....
4) The plots that are shown are to just to give you an insight.



Problem_1 Part(b)

c) Time-Dependent Part:

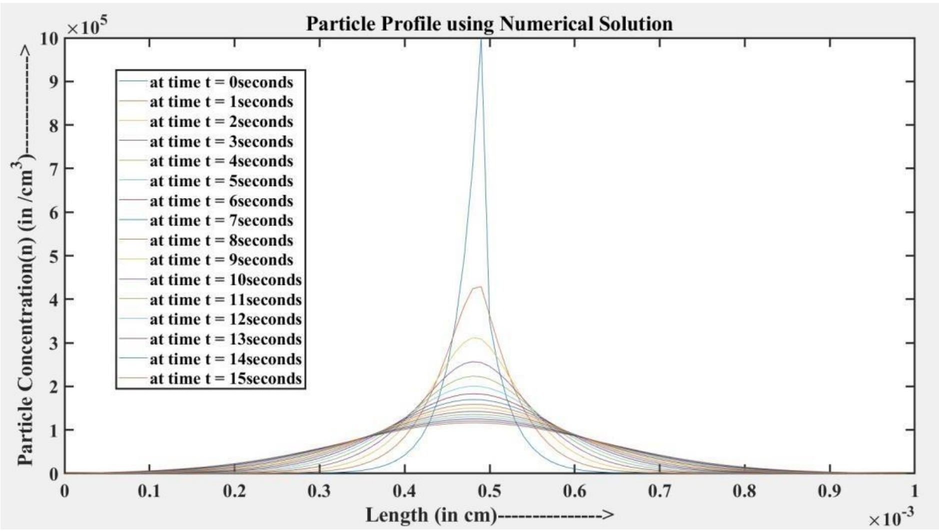
$$\frac{d^2n}{dx^2} = \frac{1}{D}\frac{dn}{dt}$$

Assume that particles are injected midway at **x=5µm** such that the density is (1+XX)*$\mathbf{10^6 cm^{-3}}$ {where, XX= last 2-digits of Roll No.} (i.e., the injection is a delta function in both space and time).Consider perfectly absorbing boundary conditions at **A** and **B,** at time **t** = **0.**Using the formalism described in class, plot the **evolution of particle density** with time over the specified domain. Compare with analytical results. Explore the significance of the parameter$\sqrt{Dt}$. (Use **D** = $\mathbf{10^{-4}}$ $\mathbf{cm^2}$ /s)

Plot the evolution of particle density with both **(i) Implicit method, and (ii) Explicit method** with C<0.5 & C >0.5, where C =D*Δt/Δx^2.

Time Dependence in terms of particle injection at time t = 0

Means particles at x=5um will starts decreasing with time.



Question- 2nd   Region of length $(L) = 10\mu m$ (6)

- Perfectly absorbing Boundary condn at $x = 0 = 10\mu m$ at time $= 0$.
- Particle Injection at $x = 5\mu m$; Density $= 10^6/cm^3$ (Delta func)

Given:- $D = 10^{-4}$ cm²/sec

To find:
(i) Evolution of particle density
(ii) Analytical result
(iii) Significance of $\sqrt{Dt}$

Solution: Now you also have Time-dependance.

There are 2 methods to do this question :→

A. Implicit or Backward Euler Method [Unconditionally Stable]

B. Explicit or forward Euler Method [Conditionally Stable]

↳ Condn $\left(C = \frac{D\Delta t}{\Delta x^2} < 0.5 \right)$ Should be followed.

[Ref to Read : Ch-7, VLSI Tech. , Pg-405
Read Whole Topic for Dopant Diffusion]

"Hence we will use using Implicit method, where you need not to worry about conditions for stability."

Backward Euler means you are using Backward difference formula for the calculation of $\left(\frac{dn}{dt}\right)$ term.

Equation:- Non-steady Diffusion Eqn (7)
or Diffusion Equation

$i \rightarrow$ posn Index
$j \rightarrow$ Time Index

$$D \frac{\partial^2 n}{dx^2} = \frac{\partial n}{\partial t} \rightarrow \text{(with respect to Time)}$$

(w.r. to position) Now for numerical soln

$$D\left\{\frac{n_{i-1}^{j} - 2n_i^{j} + n_{i+1}^{j}}{\Delta x^2}\right\} = \left\{\frac{n_i^{j} - n_i^{j-1}}{\Delta t}\right\}$$

Posn change. -Time change

let assume $C \Leftarrow \frac{D\,\Delta t}{\Delta x^2}$

$$\frac{D\,\Delta t}{\Delta x^2}\left\{n_{i-1}^{j} - 2n_i^{j} + n_{i+1}^{j}\right\} = n_i^{j} - n_i^{j-1}$$

Rearrange above eqn to get,

$$\boxed{n_i^{j} = \left[C\left(n_{i-1}^{j} + n_{i+1}^{j}\right) + n_i^{j-1}\right] / (2C+1)}$$

Follow:- (i) Iterate the eqn to find particle profile for each j (time)

(ii) Then iterate for j (time) to get time Evolution effect on particle profile

Problem 2: Consider a region of length 100um. Assume that the region is devoid of any particles at time t=0. Also assume perfectly absorbing boundary condition at x=100um. Solve for the diffusion of particles from the side x=0 as a function of time under the assumption that n(x=0,t)= 2000. Plot the space and temporal evolution of the particle density profile. (Note that this scenario is very similar to doping of a semiconductor to form a PN junction diode). Compare the numerical solution with the analytical solution.

Time Dependence in terms of particle injection at all times time.

Means particles at x=0 will remain constant at all times.

Comment: Same equations as mentioned on the previous page will be used.