INTRODUCTION

There are two approaches to discuss diffusion. These include Microscopic and Macroscopic view-points. In macroscopic viewpoint the overall diffusion of dopant profile is considered and how much diffusion took place is predicted. This is achieved by finding the solution of a diffusion equation based on boundary conditions. In designing of dopant profiles in semiconductor devices this approach is beneficial.

The diffusion process is described by Fick's law. Fick's first law states that the molar flux of a species is directly proportional to its concentration gradient. Constant of proportionality is D, the diffusion coefficient. Here the species of our interest is the given dopant.

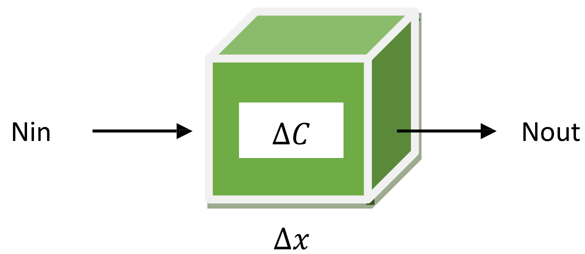
Mathematically it is defined as –

$$N = -D \frac{\partial C}{\partial X}$$

Where N is flux (in number of atoms per m^2 per sec) , D is the diffusivity (m^2/ sec) and $\frac{\partial C}{\partial X}$ is the concentration gradient.

A practically better profile of concentration with space and time is given by second law of Fick. This law is simply the conservation of mass.

Flux accumulated = Flux in – Flux out.



Which can be written as-

$$\frac{\Delta C}{\Delta t} = \frac{\Delta N}{\Delta x} = \frac{Nin - Nout}{\Delta x}$$

After substituting from Fick's first law we get :

$$\frac{\partial C}{\partial t} = \frac{\partial C}{\partial x} \left(D \frac{\partial C}{\partial x} \right)$$

If for a given temperature D is constant then we can rewrite above expression as

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

PROBLEM STATEMENT

Consider the diffusion from an infinite source of dopant on a lightly doped wafer. Find the dopant concentration profile which is changing with time and space both. Write all the assumptions you have taken with initial and boundary conditions.

Finally plot the concentration (C vs x) profile with the help of MATLAB by assuming:-

A. t = 1sec and for D = [0.1:0.1:0.5] m^2/sec
B. D = 0.1 m^2/sec and for t = [1:1:5] sec

ASSUMPTIONS AND BOUNDARY CONDITIONS

Assumptions:-

1. Diffusion profile follows Fick's 2nd law $\frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2}$
2. The diffusivity, D is constant for the process.

Boundary conditions:-

1. C = 0 at t = 0 for x>0.
2. C = C_0 at t = 0 for x< 0.

SOLUTION

Consider a series of dopant layer, each of thickness Δx and of unit cross section. Each layer initially contains a dose of CΔx dopant atoms, which in the absence of the rest of the layer would diffuse according:-

$$C(x,t) = \frac{Q}{2\sqrt{\pi D t}} e^{\left(\frac{-x^2}{4Dt}\right)}$$

Q : quantity of dopant present in the spike.

To obtain the solution for infinite source of dopant, we can make use of a simple linear superposition of solutions for each of the thin layers to give:-

$$C(x,t) = \frac{C0}{2\sqrt{\pi Dt}} \sum_{i=1}^{n} \Delta x_i \, e^{-\frac{(x-x_i)^2}{4Dt}}$$

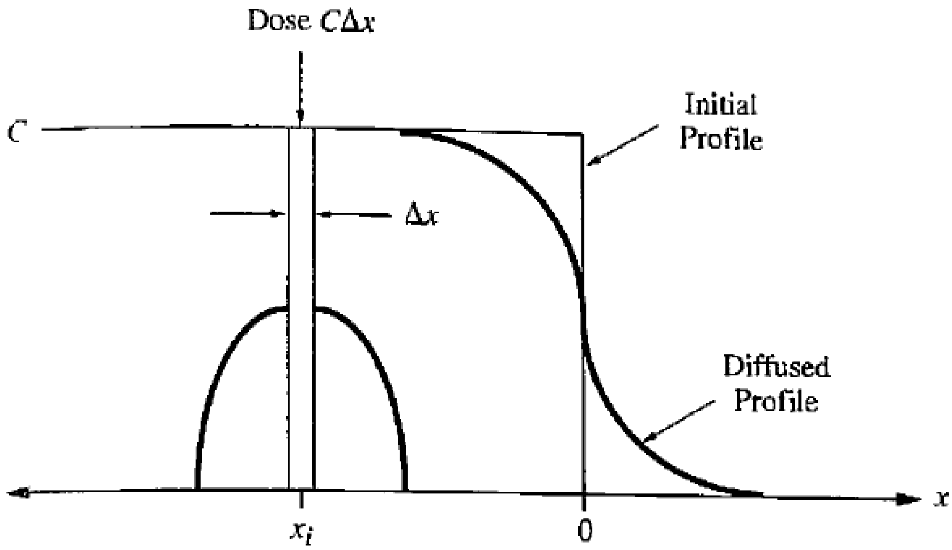


Figure 1 : Error function solution for diffusion is the sum of Gaussian functions

In the limit of thin layer, the s um becomes an integral and the solution is:-

$$C(x,t) = \frac{C0}{2\sqrt{\pi Dt}} \int_{-\infty}^{0} e^{-\frac{(x-\alpha)^2}{4D}} d\alpha$$

Let $\frac{x-\alpha}{2\sqrt{D}} = y$

And substituting gives:-

$$C(x,t) = \frac{C0}{\sqrt{\pi}} \int_{\frac{x}{2\sqrt{Dt}}}^{\infty} e^{-y^2} \, dy$$

Use the following integral definitions and properties of the error function:-

$$erfc(z) = \frac{2}{\sqrt{\pi}} \int_{z}^{\infty} e^{-y^2} dy$$

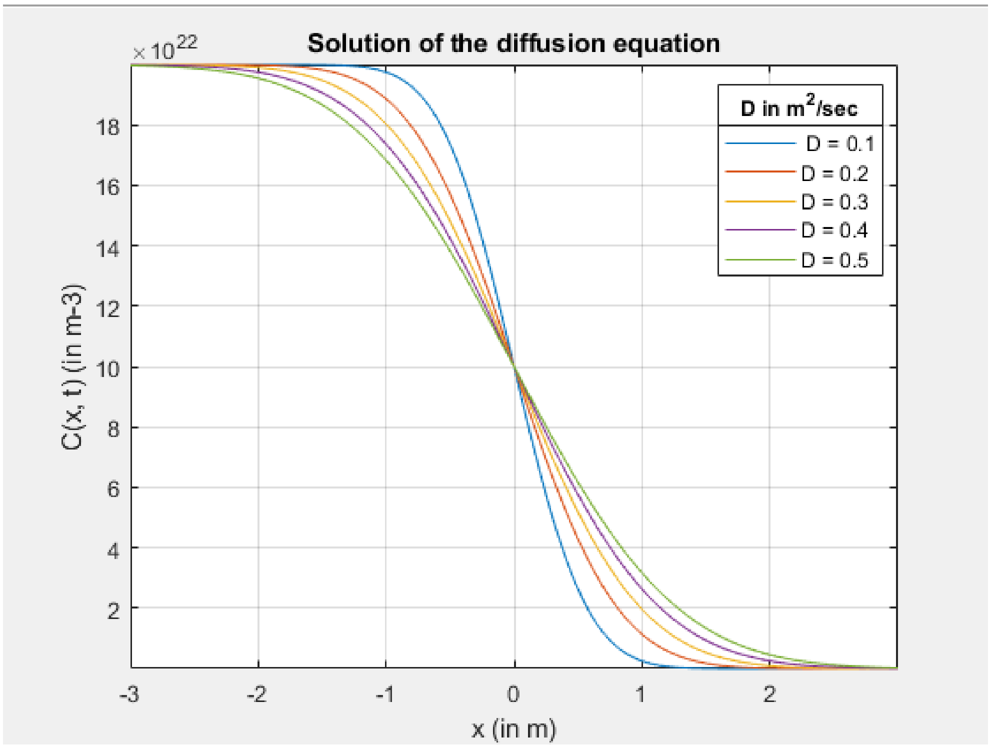
and $erf(z) + erfc(z) = 1$

Thus, the solution of the diffusion equation from an infinite source becomes:-

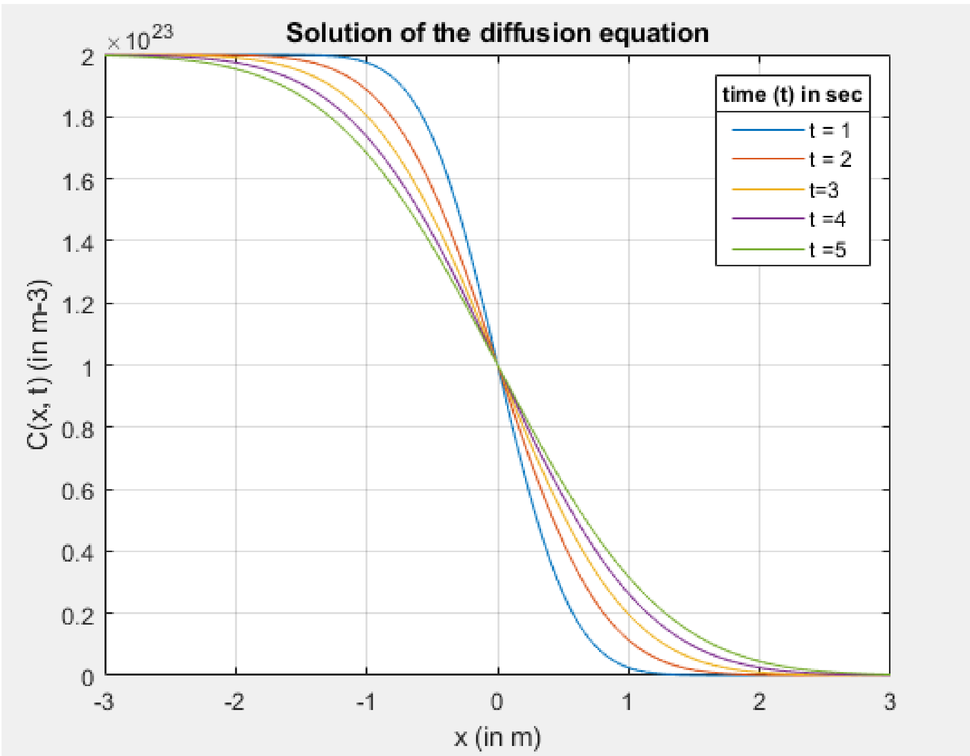
$$C(x,t) = \frac{C0}{2} \left[1 - erf\left(\frac{x}{2\sqrt{Dt}}\right) \right]$$

MATLAB PLOTS

PART A : t = 1sec and for D = [0.1:0.1:0.5] m^2/sec. (for $C_0 = 2 \times 10^{23}$ m^{-3})



PART B : D = 0.1 m^2/sec and for t = [1:1:5] sec. (for $C_0 = 2 \times 10^{23}$ m^{-3})



REFERENCES

1. Plummer, J. D., Deal, M. D., & Griffin, P. B. (2000). *Silicon VLSI technology: Fundamentals, practice, and modeling*. Upper Saddle River, NJ: Prentice Hall.
2. L.S. Darken and R.W. gurry, *physical chemistry of metals*, Mcgraw-hill 1953.