Infinite integration of the Fick's second law, $\frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial x^2}$

We have

$$c(x,t) = \frac{\alpha}{\sqrt{t}} e^{-x^2/4Dt} \qquad (2)$$

As the B diffuses into A, the total amount of B is fixed

$$\int_0^\infty c(x,t)dx = N = \text{constant}$$

Then,

$$\int_0^\infty \frac{\alpha}{\sqrt{t}} e^{-x^2/4Dt} dx = \alpha\, 2\ \sqrt{D} \quad \int_0^\infty e^{-(\frac{x}{2\sqrt{Dt}})^2} d(\frac{x}{\sqrt{Dt}}) = N$$

To solve the above equation, let's define $y = \frac{x}{2\sqrt{Dt}}$ then we have,

$$\alpha\, 2\ \sqrt{D} \quad \int_0^\infty e^{-y^2} dy \ = N$$

since $\int_0^\infty e^{-y^2} dy = \frac{\sqrt{\pi}}{2}$

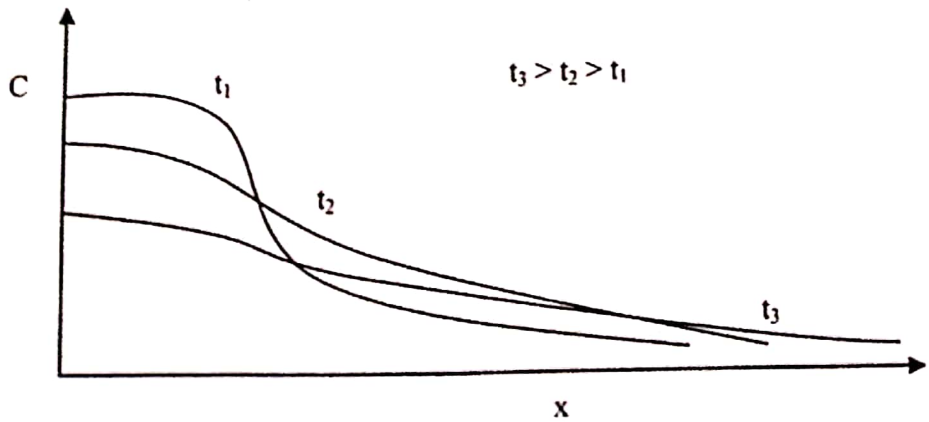
then,

$$\alpha = \frac{N}{\sqrt{\pi D}}$$

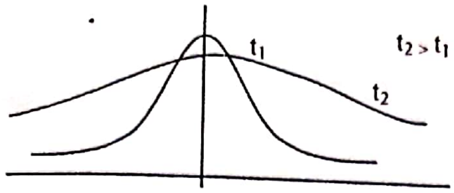
so Eq. (2) can now be written as

$$c(x,t) = \frac{N}{\sqrt{\pi D t}} e^{-x^2/4Dt} \qquad (3)$$

as determined by this diffusion kinetics equation, the concentration profile of carbon as various times will be like this



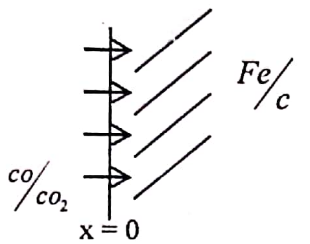
..he above diffusion is one-direction (0 → +∞). But if we extends it to two-way, from -∞ to +∞ (like a droplet dissolved into a solution) with dopant at x=0, then we have

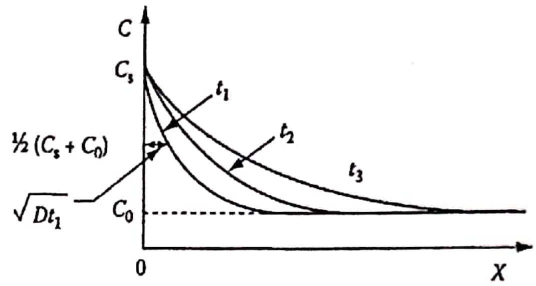


$$a = N/2\sqrt{\pi D}$$

$$c(x,t) = \frac{N}{2\sqrt{\pi D t}} e^{-x^2/4Dt}, \quad x\,(-\infty, \infty)$$

Situation b): Doping with a fixed surface concentration (e.g. carburization of steel)

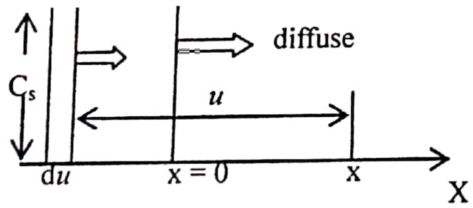




Carbon concentration profile shown at different times,

Carbonization thickness is defined as $\frac{1}{2}(c_s+c_0) = \sqrt{Dt}$

The solution of the Fick's second law can be obtained as follows, the surface is in contact with an infinite long reservoir of fixed concentration of C_s. For $x < 0$, choose a coordinate system *u*.



The fixed amount of dopant per area is $C_s\, d\mu = N$, which diffuse toward right. Then using Eq. (3) above, the slab "du" contributes to the concentration at x is

$$dc(x, t) = \frac{C_s du}{\sqrt{\pi D t}} e^{-\mu^2/4Dt}$$

So, all the slabs from x= -∞ to x totally contribute

$$c(x, t) = \int_x^\infty dc(x,t) = \int_x^\infty \frac{C_s}{\sqrt{\pi D t}} e^{-\mu^2/4Dt} d\mu$$

Defining $y = \frac{\mu}{2\sqrt{Dt}}$, then,

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

$$= \frac{2c_s}{\sqrt{\pi}} \left[\int_0^{\infty} e^{-y^2} dy - \int_0^{x/2\sqrt{Dt}} e^{-y^2} dy \right]$$

$$= \frac{2c_s}{\sqrt{\pi}} \left[\frac{\sqrt{\pi}}{2} - \int_0^{x/2\sqrt{Dt}} e^{-y^2} dy \right]$$

$$= c_s \left[1 - \text{erf}\left(\frac{x}{2\sqrt{Dt}} \right) \right]$$

Where *error function* $\text{erf}(z) = \frac{2}{\sqrt{\pi}} \int_0^{z} e^{-y^2} dy$

Considering boundary conditions:

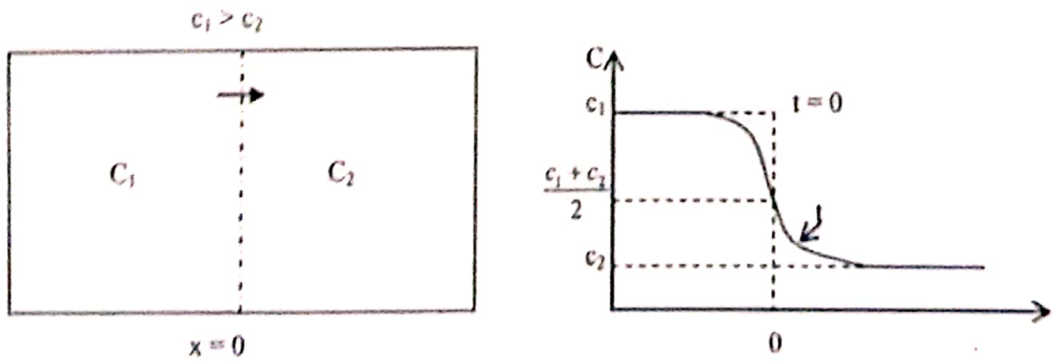
$c(x = 0) = c_s$,

$c(x = \infty) = c_0$, corresponding to the original concentration of carbon existing in the phase, c_0 remains constant in the far bulk phase at $x = \infty$.

$$c(x,t) = c_s - (c_s - c_0)\,\text{erf}\left(\frac{x}{2\sqrt{Dt}} \right)$$

the concentration profile shown above follows this diffusion equation.

Now let's consider Interdiffusion as shown below, which represents more general cases.



Solving the Fick's second law gives

$$c(x,t) = \left(\frac{c_1 + c_2}{2} \right) - \left(\frac{c_1 + c_2}{2} \right) \text{erf}\left(\frac{x}{2\sqrt{Dt}} \right)$$

Interdiffusion is popular between two semi-infinite specimens of different compositions c_1, c_2, when they are joined together and annealed, or mixed in case of two solutions (liquids). Many examples in practice fall into the case interdiffusion, including two semiconductor interface, metal-semiconductor interface, etc.