CHE323/CHE384
Chemical Processes for Micro- and Nanofabrication
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# Lecture 14
# Diffusion, part 2

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**Reading**:
Chapter 3, *Fabrication Engineering at the Micro- and Nanoscale*, 4th edition, Campbell





## Solving the Diffusion Equation

- To solve the diffusion equation, we need
  - One initial condition
  - Two boundary conditions for each dimension
  - Knowledge of the diffusivity D(x,y,z,t) or D(C)
- We'll assume D = constant here, and 1D

$$\frac{\partial C(z,t)}{\partial t} = \frac{\partial}{\partial z}\left(D\frac{\partial C(z,t)}{\partial z}\right) = D\frac{\partial^2 C}{\partial z^2}$$





## Case 1: Constant Source

- Initial and boundary conditions
  - $C(0,t) = C_s$ (concentration at top is constant)
  - C(z,0) = 0 for z > 0 (initial condition)
  - C(∞,t) = 0
- Solution:

$$C(z,t) = C_s erfc\left(\frac{z}{2\sqrt{Dt}}\right), \qquad t > 0$$

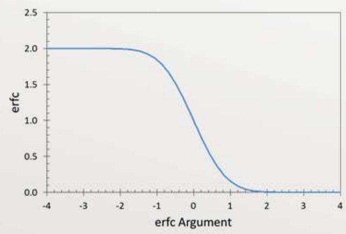
$\sqrt{Dt}$ = diffusion length (average distance a dopant moves)





## Complimentary Error Function

$$erfc(\theta) = \frac{2}{\pi}\int_\theta^\infty e^{-y^2}dy = 1 - erf(\theta)$$




$erfc(0) = 1$

$erfc(0.5) = 0.4795$

$erfc(\infty) = 0$

$C(z,t) = C_s erfc\left(\frac{z}{2\sqrt{Dt}}\right)$

See Appendix V of Campbell for properties and table





## Dopant Dose

- The "total dose", $Q_T$, is the total number of dopants per unit area

$$Q_T(t) = \int_0^\infty C(z,t)dz$$

- For the constant source case,

$$Q_T(t) = \frac{2}{\pi}C_s\sqrt{Dt}$$





## Case 2: Limited Source
(drive-in diffusion)

- Initial and boundary conditions
  - C(z,0) = 0, z > 0
  - dC(0,t)/dt = 0 (no flux at top)
  - C(∞,t) = 0
  - Constant dose: $\int_0^\infty C(z,t)dz = Q_T = constant$
- Solution:

$$C(z,t) = \frac{Q_T}{\sqrt{\pi Dt}}e^{-z^2/4Dt}, \qquad t > 0$$

## Case 3: Buried Gaussian Source

- Initial and boundary conditions
  - Gaussian: $C(z,0) = \frac{Q_T}{\sqrt{2\pi\sigma_o^2}} e^{-(z-\mu)^2/2\sigma_o^2}, \quad z \ge 0, \mu \gg \sigma_o$
  - dC(0,t)/dt = 0 (no flux at top)
  - C(∞,t) = 0
- Solution: $\sigma^2 = \sigma_o^2 + 2Dt$ ($\sqrt{2Dt}$ = diffusion length)

$$C(z,t) = \frac{Q_T}{\sqrt{2\pi\sigma^2}} e^{-(z-\mu)^2/2\sigma^2}, \quad z \ge 0, t \ge 0$$





## When Can We Use These Solutions?

- Case 1: Constant Source
  - Classic old-style diffusion
- Case 2: Limited Source
  - Drive in diffusion: dopant dose deposited at the top of the wafer (within a depth $\ll \sqrt{Dt}$)
- Case 3: Buried Gaussian
  - Ion implantation resulted in Gaussian distribution buried within the wafer





## Lecture 14: What have we learned?

- What are the cases where we have derived simple analytical solutions to the diffusion equation?
- What assumptions did we have to make in order to derive our solutions?
- When might these solutions be useful?