

Module 2 :

“Diffusive” heat and mass transfer

Lecture 10:

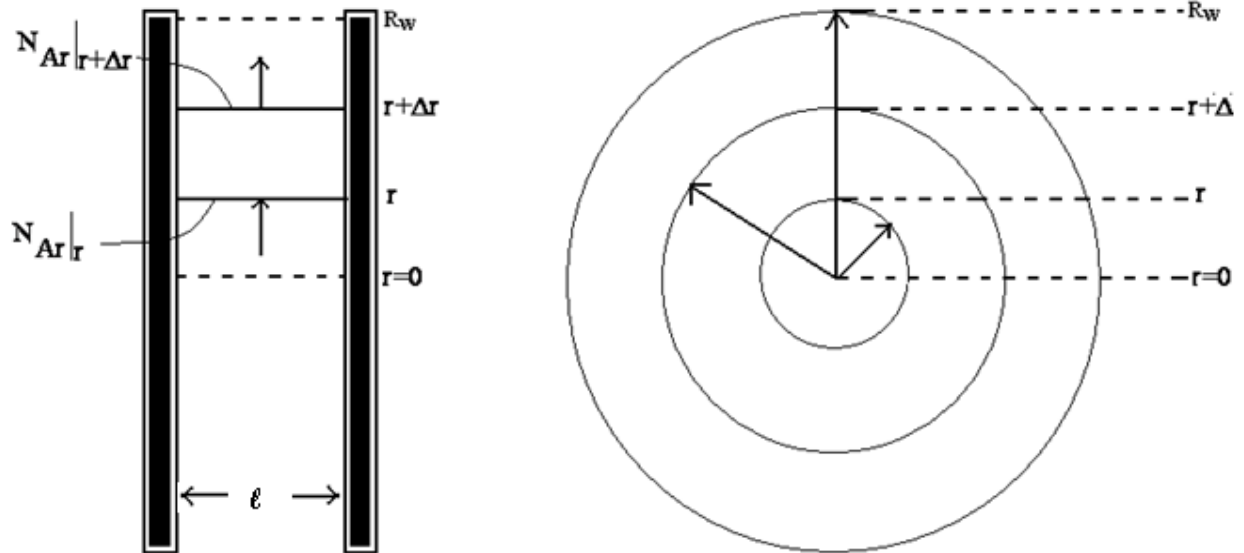
Simultaneous Mass Diffusion and

Reaction between wafers in Low

Pressure Chemical Vapor Deposition

Mathematical Model for Mass Transfer with Chemical Reaction: Diffusion-Reaction

Equation



Writing general mass balance

$$\text{In} - \text{Out} + \text{Generation} = 0$$

Shell mass balance on SiH_2 (A)

Writing for component A, we have

$$N_{Ar} (2\pi r) - N_{Ar} (2\pi r)_{r+\Delta r} + 2(2\pi r \Delta r r_A'') = 0 \quad (10.1)$$

where N_{Ar} is the flux of A at r and r_A'' is the rate of reaction

The factor two in the last term of the balance equation implies that the deposition is been carried out on both wafer faces. Dividing equation (10.1) by $2r\pi$ and taking limit $\Delta r \rightarrow 0$ we get

$$\frac{1}{r} \frac{d(N_{Ar}r)}{dr} = \frac{2}{l} r_A \quad (10.2)$$

Now, for binary diffusion (A&B) the molar flux is given by

$$N_{Ar} = -c D_{AB} \frac{dx_A}{dr} + x_A (N_{Ar} + N_{Br}) \quad (10.3)$$

where D_{AB} is the diffusivity of A in B

For every molecule of A diffusing in, however, one molecule of B diffuse out. This is the case of equimolar counter diffusion. For which we can write

$$N_{Ar} = -N_{Br}$$

hence equation (10.3) becomes

$$N_{Ar} = -c D_{AB} \frac{dx_A}{dr} \quad (10.4)$$

Assuming constant c (which means that $P/RT = \text{const}$, for ideal gas)

$$N_{Ar} = -D_{AB} \frac{dc_A}{dr} \quad (10.5)$$

Also, for first order reaction

$$-r_A'' = k C_A \quad (10.6)$$

Using equations (10.5) and (10.6) in (10.2) we get

$$\frac{1}{r} \frac{d}{dr} \left(r \frac{dc_A}{dr} \right) - \frac{2k}{D_{AB}} \frac{c_A}{l} = 0 \quad (10.7)$$

Note that equation (10.7) can also be derived using General Mass balance equation.

Boundary Conditions

$$c_A = c_{A0} \quad \text{at } r = R_w$$

$$\frac{dc_A}{dr} = 0 \quad \text{at } r = 0$$

Defining dimensionless quantities

$$\theta = \frac{c_A}{c_{A0}} \quad \text{and} \quad J = \frac{r}{R_w}$$

Then after inserting the dimensionless quantities in equation (10.7), we get

$$\frac{1}{J} \frac{d}{dJ} \left(J \frac{d\theta}{dJ} \right) - \phi_1^2 \theta = 0 \quad (10.8)$$

$$\text{where } \phi_1 = \sqrt{\frac{2kR_w^2}{D_{AB} l}} \quad [\text{which is analogous to } N \text{ in equation for rectangular fin}]$$

For equation (10.8) the new B.Cs are

$$\text{At } J = 0 \quad \frac{d\theta}{dJ} = 0 \text{ and}$$

$$\text{At } J = 1 \quad \theta = 1$$

Then the solution to equation (10.8) is given by

$$\theta = AI_0(\phi_1 J) + BK_0(\phi_1 J) \quad (10.9)$$

Where

I_0 is a modified Bessel function of the first kind of order zero and;

K_0 is a modified Bessel function of the second kind of order zero

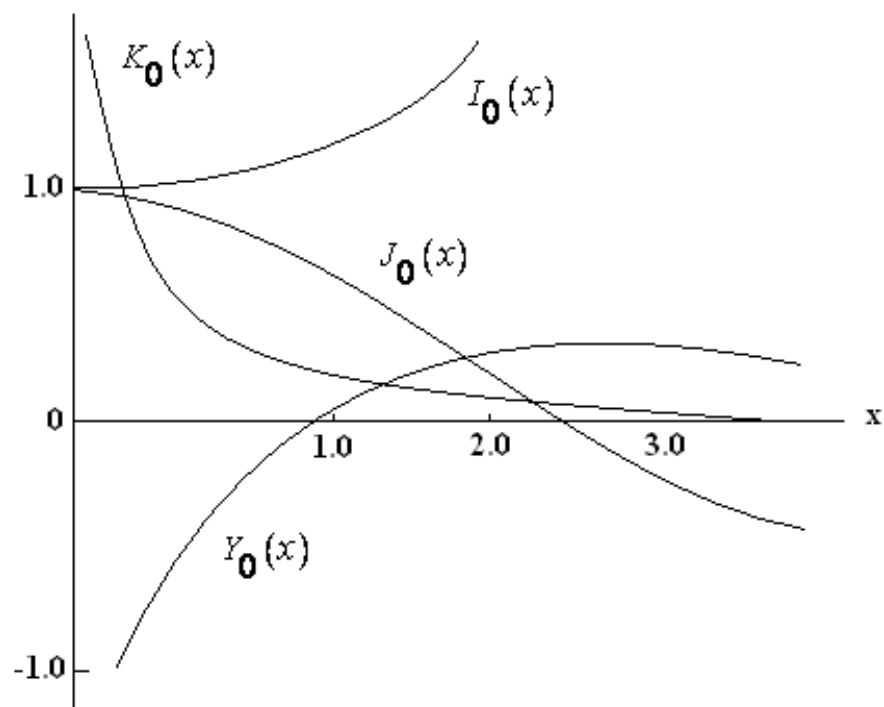


Fig.10.2 Bessel function of zero order

Since $K_0(0) \rightarrow \infty$ therefore $B = 0$

Then equation (10.14) becomes

$$\theta = \frac{c_A}{c_{A0}} = \frac{I_0(\phi_1 J)}{I_0(\phi_1)} \quad (10.10)$$

Effectiveness factor

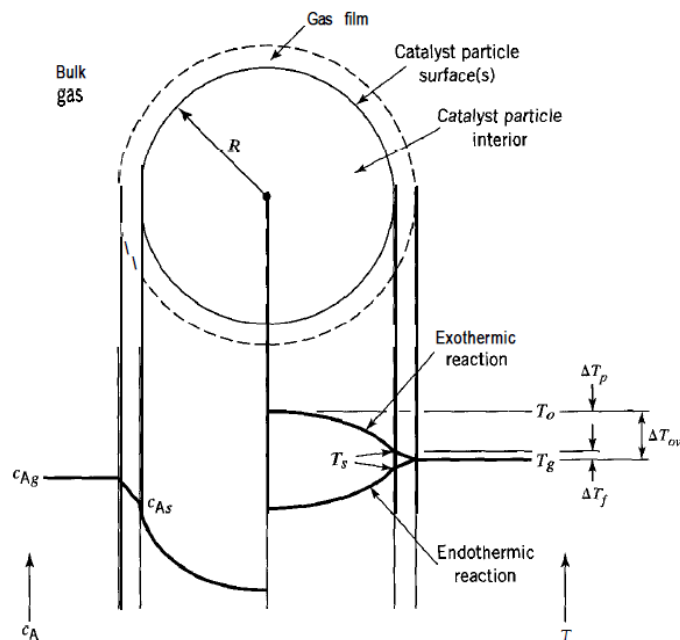


Fig.10.3 Temperature and Concentration gradients in porous catalyst particle

Since concentration and temperature varies from point to point within a catalyst particle, shown in Fig.(10.3), the rate of reaction varies accordingly. In other words, we can say that the effectiveness of the catalyst varies within the particle.

For this purpose, the term effectiveness factor η , which can be defined as the ratio of the actual rate of reaction for the particle as a whole to the intrinsic rate at the surface conditions, C_{As} and T_s . In terms of reactant A

$$\eta = \frac{\text{Actual dissipation rate}}{\text{deposition rate if } c_A \text{ was equal to } c_{A_0} \text{ throughout inter Wafer space}}$$

$$\eta = \frac{-(N_{Ar})_{r=R_w} (2R_w \pi l)}{2R_w^2 \pi (-r_{Ao} ")} \quad (10.11)$$

Adjusting the parameters and using dimensionless quantities

$$\eta = 2 \frac{\left(\frac{d\theta}{dJ} \right)_{J=1}}{\Phi_1^2} \quad (10.12)$$

Therefore from equations (10.10) and (10.12), we get

$$\eta = \frac{2 I_1(\phi_1)}{\phi_1 I_0(\phi_1)} \quad (10.13)$$

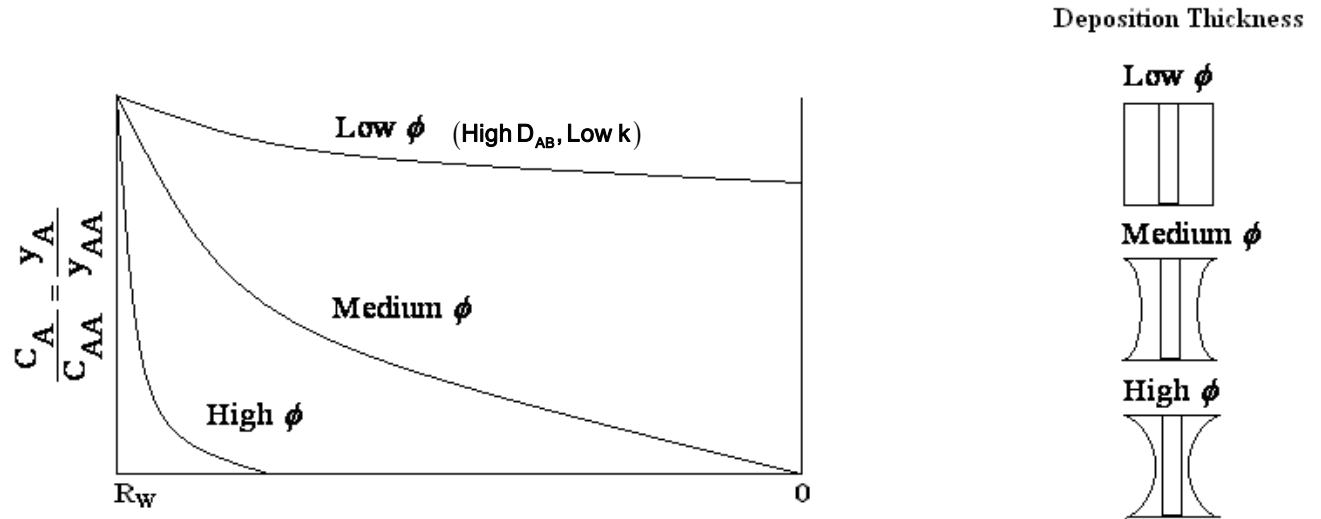


Fig. 10.4 Deposition of film thickness for different ϕ