DEPARTMENT OF MECHANICAL ENGINEERING

AGUS PULUNG SASMITO

Problem statement

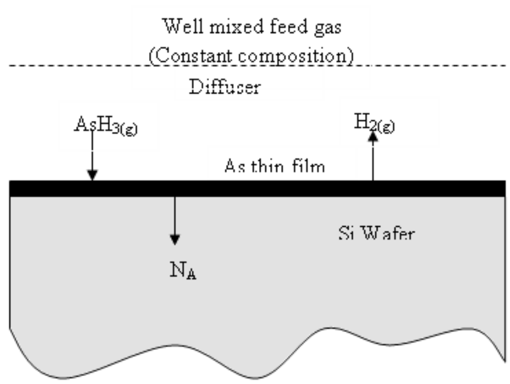
Problem

In the manufacture of semi conducting thin films, a thin film of solid arsenic is laid down onto the surface of a silicon wafer by the diffusion-limited chemical vapor deposition of arsine, AsH_3.

$$2AsH_{3(g)} \rightarrow 2As_{(s)} + 3H_{2(g)}$$

The gas headspace 5 cm above the surface of the wafer is stagnant. Arsenic atoms deposited on the wafer surface then diffuse into the solid silicon to "dope" the wafer and impart semiconducting properties to the silicon, as shown in the figure bellow. The process temperature is 1050°C. The diffusion coefficient of arsenic in silicon is 5×10^{-13} cm^2/s at this temperature, and the maximum solubility of arsenic in the silicon is 2×10^{21} atoms/cm^3. the density of solid silicon is 5×10^{22} atoms/cm^3. Since the diffusion coefficient is so small, the arsenic atoms do not "penetrate" very far into the silicon solid, usually less than a few microns. Consequently, a relatively thin silicon wafer can still be considered as a "semi-infinite" medium for diffusion. In this problem, consider the solid silicon as the system for analysis.

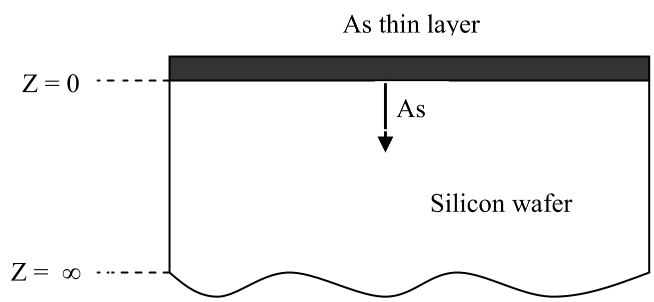
a) State at least five reasonable assumptions for the mass-transfer aspects of the doping process. What coordinate system should be used?
b) What is the simplified form of the general differential equation for mass transfer in terms of the arsenic concentration within the silicon? Propose reasonable boundary and initial condition that maybe used to solve the resulting differentia equation.



Solution

Known: Temperature 1050^0C, Diffusion coefficient As in Si 5 x 10^{-13}cm^2/s, maximum solubility As in Si 2 x 10^{21} atoms/cm^3, density silicon 5 x 10^{22}atoms/cm^3.

a) Assumption:
   1) Rate of reaction $2AsH_{3(g)} \rightarrow 2As_{(s)} + 3H_{2(g)}$ is very fast compared to As diffuse into silicon wafer (diffusion coefficient 5 x 10^{-13} cm^2/s). So, if the solid silicon is the system for analysis, the reaction and transport gas AsH_3 can be neglected for system analysis.
   2) The thickness of As thin film compare to the depth of the As diffuse to silicon wafer, which is only a few micron, is very large. So the As thin film can be assumed as As source and silicon wafer as sink.
   3) Since diffusivity of As in silicon wafer is very small, then the concentration of As thin film is very small change. Then, As concentration at surface (z = 0) can be assumed as constant.
   4) Since diffusion only takes place on the z direction (x and y contribute very small compare to z direction) so, the diffusion can be assumed as 1 dimension.
   5) There is no homogenous reaction within diffusion zone.
   6) Since the diffusion coefficient is very small, the arsenic atoms do not diffuse very far into the silicon solid. then, the silicon wafer can be considered as a "semi-infinite" medium for diffusion
   7) Coordinate to be used is Cartesian coordinate.



$T = 1050^0C$
$D_{As\text{-}Si} = 5.10^{-13} cm^2/s$
$S_{As\ in\ Si,\ max} = 2.10^{21}$ atoms/cm^3
$\rho_{Si} = 5.10^{22}$ atoms/cm^3

b) General differential equation and boundary condition

$$\nabla \cdot \mathbf{N_A} + \frac{\partial C_A}{\partial t} - R_A = 0 \tag{1}$$

where

$$\mathbf{N_A} = -cD_{AB}\nabla y_A + c_A\mathbf{V} \tag{2}$$

then

$$-\nabla cD_{AB}\nabla y_A + \nabla \cdot c_A\mathbf{V} + \frac{\partial C_A}{\partial t} - R_A = 0 \tag{3}$$

since there is no reaction and no mass transfer due to fluid motion

$$-\nabla cD_{AB}\nabla y_A + \frac{\partial C_A}{\partial t} = 0 \tag{4}$$

And diffusion coefficient is constant

$$-D_{AB}\nabla^2 C_A + \frac{\partial C_A}{\partial t} = 0 \tag{5}$$

or

$$\frac{\partial C_A}{\partial t} = D_{AB}\frac{\partial^2 C_A}{\partial x^2} + D_{AB}\frac{\partial^2 C_A}{\partial y^2} + D_{AB}\frac{\partial^2 C_A}{\partial z^2} \tag{6}$$

and assumed that the diffusion only takes place at z direction, then

$$\frac{\partial C_A}{\partial t} = D_{AB}\frac{\partial^2 C_A}{\partial z^2} \tag{7}$$

Initial and boundary conditions:

For semi-infinite medium,

i. At t = 0, $C_A(z,0) = C_{As0} = 0$ for all z (initial condition)
ii. At z = 0, $C_A(0,t) = C_{As}$, for $t > 0$,
    where C_{As} = surface concentration 2.10^{21} atoms/cm^3
iii. At $z = \infty$, $C_A(\infty,0) = C_{As0} = 0$ for all t

Then, the analytical solution of $\frac{\partial C_A}{\partial t} = D_{AB}\frac{\partial^2 C_A}{\partial z^2}$ at the stated initial and boundary condition can be obtained by Laplace transform technique.

where $\theta = C_A - C_{AS0}$ then

$$\frac{\partial \theta}{\partial t} = D_{AB}\frac{\partial^2 \theta}{\partial z^2} \tag{8}$$

with $\theta(z,0) = 0$

$\theta(0,t) = C_{As} - C_{As0}$

$\theta(\infty,t) = 0$

Then laplace transform of eq (8) with respect to time

$$s\overline{\theta} - 0 = D_{AB}\frac{d^2\overline{\theta}}{dz^2} \tag{9}$$

Which readily transform to ODE

$$\frac{d^2\overline{\theta}}{dz^2} - \frac{s}{D_{AB}}\overline{\theta} = 0 \tag{10}$$

With transformed boundary

$$\overline{\theta}(z=0) = \frac{C_{As} - C_{As0}}{s} \tag{11}$$

And

$$\overline{\theta}(z=\infty) = 0$$

The general analytical solution is

$$\bar{\theta} = A_1 e^{+\sqrt{s/D_{AB}}z} + B_1 e^{-\sqrt{s/D_{AB}}z} \quad (12)$$

The boundary condition at z = ∞ requires integration constant A_1 =0, while boundary condition at z = 0 requires

$$B_1 = \frac{C_{As} - C_{As0}}{s}$$

Then, the general analytical solution reduces to

$$\bar{\theta} = \frac{(C_{As} - C_{As0})}{s} e^{-\sqrt{s/D_{AB}}z} \quad (13)$$

The inverse Laplace transform

$$\bar{\theta} = (C_{As} - C_{As0}) erfc\left(\frac{z}{2\sqrt{D_{AB}t}}\right) \quad (14)$$

or

$$\frac{C_{As}(z,t) - C_{As0}}{(C_{As} - C_{As0})} = erfc\left(\frac{z}{2\sqrt{D_{AB}t}}\right) = 1 - erf\left(\frac{z}{2\sqrt{D_{AB}t}}\right) \quad (15)$$

By substituting boundary condition

$$\frac{C_{As}(z,t) - 0}{(2.10^{21} - 0)} = 1 - erf\left(\frac{z}{2\sqrt{D_{AB}t}}\right) \quad (16)$$

$$C_{As}(z,t) = 2.10^{21}\left(1 - erf\left(\frac{z}{2\sqrt{5.10^{-13}t}}\right)\right) \quad (17)$$