MSEG201 Homework 5

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Steady State Diffusion

This can be solved using Fick's First law of diffusion:

$$J = -D\frac{dC}{dx}$$

This can be rearranged for the concentration gradient and solved for the high-pressure concentration

$$\frac{dC}{dx} = -\frac{J}{D}$$

$$dC = C_{\text{high-pressure}} - C_{\text{low-pressure}} = + \frac{J}{D} dx$$

$$C_{\text{high-pressure}} = C_{\text{low-pressure}} + \frac{J}{D}dx$$

Now plugging in the given values:

$$C_{\rm high-pressure} = 0.5\,{\rm kg/m}^3 + (0.002\,{\rm m})\,\frac{2.48\times 10^{-8}\,\,{\rm kg/m}^2{\rm s}}{4.50\times 10^{-11}\,\,{\rm m}^2/{\rm s}} = 1.60\,{\rm kg/m}^3$$

Diffusion of Aluminum in Silicon

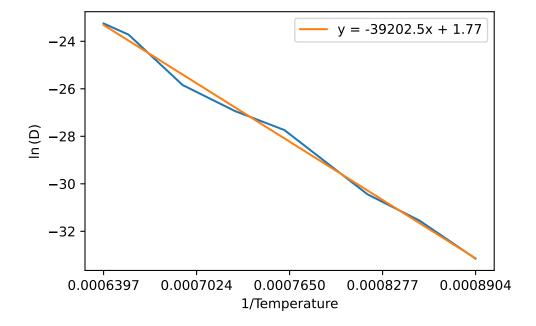
```
import numpy as np
import matplotlib.pyplot as plt

diffusivity = np.array([8e-11, 5e-11, 6e-12, 2e-12, 9e-13, 6e-14, 2e-14, 4e-15])
temperature = np.array([1290, 1250, 1170, 1100, 1040, 950, 900, 850]) + 273.15
```

```
x = 1/temperature
y = np.log(diffusivity)
m,b = np.polyfit(x,y,1)

fig, ax = plt.subplots()

ax.plot(x,y)
ax.plot(x,m*x+b, label=f'y = {m:.1f}x + {b:.2f}')
ax.set_xlabel('1/Temperature')
ax.set_ylabel('$\ln$(D)')
ax.set_ylabel('$\ln$(D)')
ax.set_xticks(np.linspace(x.min(), x.max(), 5))
ax.legend()
```



a)

This has effectively plotted $\ln(D)=\ln(D_0)+\frac{1}{T}\left(\frac{-Q_d}{R}\right)$. The intercept is $\ln(D_0)$, so $D_0=\exp(b)=58.4$. The slope is $\frac{-Q_d}{R}$, so $Q_d=-mR=-(-39202)(8.6173\times 10^{-5})=3.38$ eV

b)

Going back to the equation

$$\ln(D(T=1000^{\circ}C)) = -39202.5 \times (1000 + 273.15)^{-1} + 1.77 = -29.02$$

$$D = \exp(-29.02) = 2.48 \times 10^{-13}$$

Doping and Diffusion

First we need to find D!

$$D = 2.14 \times 10^{-5} \exp \left[\frac{3.65}{(8.62 \times 10^{-5})(1200 + 273.15)} \right]$$

$$D = 6.509 \times 10^7$$

Now rearranging the thin source solution

$$\frac{C\sqrt{\pi Dt}}{B} = \exp\left[\frac{-x^2}{4Dt}\right]$$

$$x = -4Dt\sqrt[2]{\ln\left[\frac{C\sqrt{\pi Dt}}{B}\right]}$$

$$x = -4(6.509 \times 10^7)(1.75 \times 3600) \sqrt[2]{\ln \left[\frac{3.63 \times 10^{17} \sqrt{\pi (6.509 \times 10^7)(1.75 \times 3600)}}{5.2 \times 10^3} \right]}$$

Carburization

a)

It matches up with the semi-infinite bar solution since there is in initial concentration throughout the system, and the diffusion takes place on mostly the first 4mm and hopefully the gear is much thicker than 4mm.

b)

Remembering the semi-infinite bar solution and reorganizing for t

$$\frac{C(x,t) - C_0}{C_s - C_x} = 1 - \operatorname{erf}\left(\frac{x}{2\sqrt{Dt}}\right)$$

$$\operatorname{erf}\left(\frac{x}{2\sqrt{Dt}}\right) = 0.75$$

And using wolfram alpha for the inverse erf

$$\frac{x}{2\sqrt{Dt}} = 0.8134$$

$$t = \frac{1}{D} \left[\frac{x}{2 \times 0.8134} \right]^2$$

finding D

$$D = D_0 \exp\left(\frac{-Q}{RT}\right) = 2.5 \times 10^{-5} \exp\left(\frac{-1.48 \times 10^5}{8.314 \times 1373}\right) = 5.851 \times 10^{-11} \, \mathrm{m^2/s}$$

and finally plugging in

$$t = \frac{1}{5.851 \times 10^{-11} \,\mathrm{m}^2/\mathrm{s}} \left[\frac{0.004 \,\mathrm{m}}{2 \times 0.8134} \right]^2 = 103328.84 \,\mathrm{sec}$$

and into the right units

$$103328.84 \sec \times \frac{1 \text{ hour}}{3600 \sec} = 28.70 \text{ hours}$$

c)

```
import numpy as np
import matplotlib.pyplot as plt
from scipy.special import erf

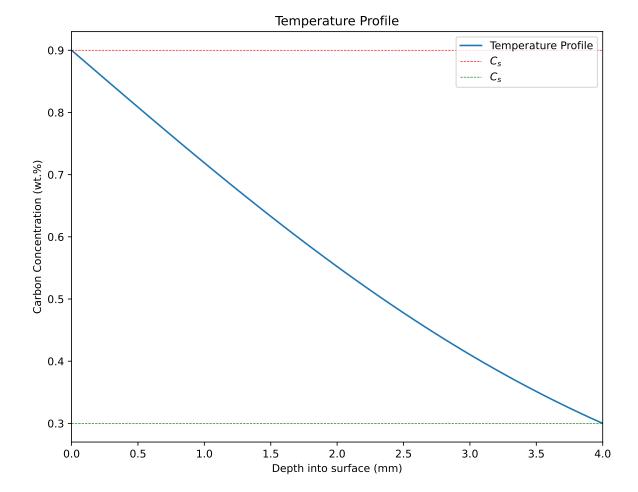
C_0 = 0.10
C_S = 0.90
t = 103328.840 # seconds!
D = 5.851e-11
```

```
x = np.linspace(0,4,100)
y = (1 - erf((x/1000) / (2 * np.sqrt(D*t))))*(C_S - C_0) + C_0

fig,ax = plt.subplots(figsize=(9,7), dpi=100)

ax.plot(x,y, label='Temperature Profile')
ax.set_xlabel('Depth into surface (mm)')
ax.set_ylabel('Carbon Concentration (wt.%)')
ax.set_xlim(0,4)
ax.hlines(0.9, 0,4, color='red', label='$C_s$', linestyle='--', linewidth=0.6)
ax.hlines(0.3, 0,4, color='green', label='$C_s$', linestyle='---', linewidth=0.6)
ax.legend()
ax.set_title('Temperature Profile')
```

Text(0.5, 1.0, 'Temperature Profile')



d)

Now D is

$$D = 2.5 \times 10^{-5} \exp\left(\frac{-1.48 \times 10^5}{8.314 \times 973}\right) = 2.834 \times 10^{-13} \,\mathrm{m}^2/\mathrm{s}$$

so the time is

$$t = \frac{1}{(2.834 \times 10^{-13} \,\mathrm{m^2/s}) \,(3600)} \left[\frac{0.004 \,\mathrm{m}}{2 \times 0.8134} \right]^2 = 5926 \,\mathrm{hours}$$