Chapter 6 - Diffusion

Topics to be covered include:

- **Diffusion mechanisms**
  - ____________
  - ____________
- **Governing equations of diffusion**
  - ______________
  - ______________
- **Influence of temperature and species**

Chapter 6 (continued)

Qualitative Questions

26 Describe the difference between kinetics and thermodynamics and explain the diffusion process in these terms.

27 Describe vacancy and interstitial diffusion. Include the types of elements involved, and their typical relative rates.

28 Explain the concepts of steady-state and nonsteady-state diffusion.

Chapter 6 (continued)

Quantitative Questions

7 Be able to apply the equation for Fick's first law, relating diffusion flux, diffusion coefficient and concentration gradient

8 Be able to apply the solution to Fick's second law for a semi-infinite solid fixed a fixed concentration at the surface (The solution given by Equation 5.5)

9 Be able to apply the concept of activation energy and the effect of temperature on diffusion

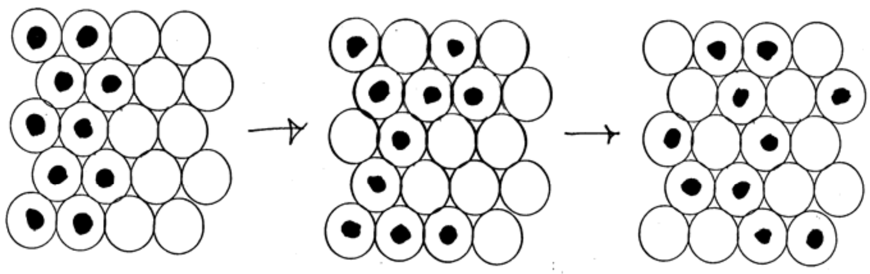
Chapter 6 (continued)

Definitions:

- ________ - Material transport by ________________________. The stepwise migration of atoms.
- _____________ - Diffusion of ___________________________.
- _____________ - Diffusion of atoms in a lattice of the same type. This consists of atoms swapping positions with vacancies and with each other.

Chapter 6 (continued)

If the system is closed, diffusion will result in a ___________ ________________, ie. the system will be ________________



Chapter 6 (continued)

Diffusion mechanisms

- **For an atom to move positions two conditions must be met:**
  - **the ________________ must be _________**
  - **the atom must have sufficient energy to break the bonds its neighbors and to squeeze through to the site**
- **Only a ______________________ have sufficient energy to do this. The fraction ___________________________.**

Chapter 6 (continued)

Diffusion mechanisms (cont.)

- **There are two mechanisms by which the movement can occur in metallic diffusion**
  - **___________ diffusion**
  - **___________ diffusion**

Chapter 6 (continued)

Diffusion mechanisms (cont.)

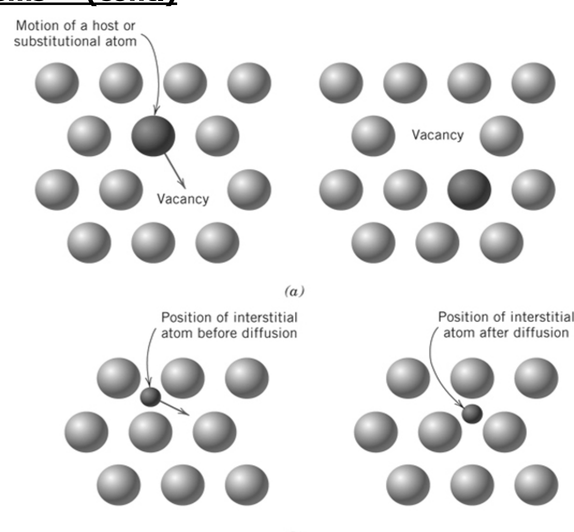


Figure 6.3

Chapter 6 (continued)

Diffusion mechanisms (cont.)

Vacancy diffusion

- **Movement of an atom into an ___________________________.**
- **There are more vacancies at _________________. (Eqn 5.1)**
- **Both self-diffusion and interdiffusion can occur by this mechanism.**

Chapter 6 (continued)

Diffusion mechanisms (cont.)

Interstitial diffusion

- **The movement of an atom from an _______________ to an adjacent one.**
- **Occurs with interstitial impurity atoms such as __________ .**
- **Occurs ________________ than vacancy diffusion. There are many more interstitial sites than vacant sites.**

Chapter 6 (continued)

Governing Equations of Diffusion

- ____________________ tells us that when two metals are in contact that there will be a _________________________ (diffusion) from ___________________________________ .
- It does not tell us, however, ___________________________ .
- __________ tells us the_____ at which the diffusion will occur. Diffusion is a __________________________ .

Chapter 6 (continued)

Governing Equations of Diffusion (cont.)

- We are interested in the rate process for two situations.
  - ________________ diffusion
  - ________________ diffusion
- **Definition**:
- steady-state - ____________ in the condition of ___________ ________________ as a function of time.
- It is important to not confuse ___________________________ .

Chapter 6 (continued)

Governing Equations of Diffusion (cont.)

Steady-state diffusion

- **The term that defines the diffusion rate is _______________ , defined as a ________________________ .**
- **Sample units**

where J = the flux

Chapter 6 (continued)

Governing Equations of Diffusion (cont.)

Steady-state diffusion (cont.)

- **At steady-state the flux is _____________________________ _____________ . This is termed Fick's first law.**

where D = the proportionality constant termed the diffusion coefficient (m^2/s)
dC/dx = the concentration gradient

Chapter 6 (continued)

Governing Equations of Diffusion (cont.)

Steady-state diffusion (cont.)

- **D is a function of the:**
  - **_______________________ (vacancy versus interstitial) ,**
  - **_________________ ,**
  - **_______________________ ,**
  - **________________ .**
- **The concentration gradient (dC/dx) is the _______________ for mass transfer.**

Chapter 6 (continued)

Governing Equations of Diffusion (cont.)

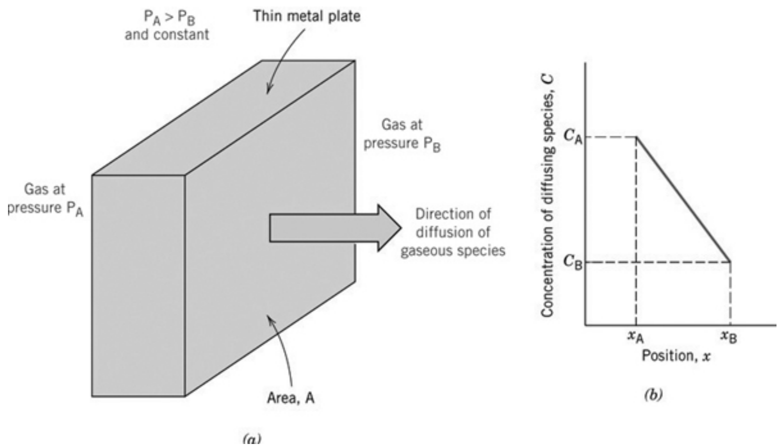
Steady-state diffusion (cont.)

- **Typically the gradient can be assumed to be _____________ ______________ . Therefore**
- **The concentration can be expressed as mass/volume, mole/volume, or directly as weight fraction.**
- **(see Example Problem 6.1)**

Chapter 6 (continued)

Governing Equations of Diffusion (cont.)

Steady-state diffusion (cont.)



Chapter 6 (continued)

Governing Equations of Diffusion (cont.)

nonsteady-state diffusion

- **Often the diffusion is ________________.**
- **In this case the flux is a ________________ ________________ .**

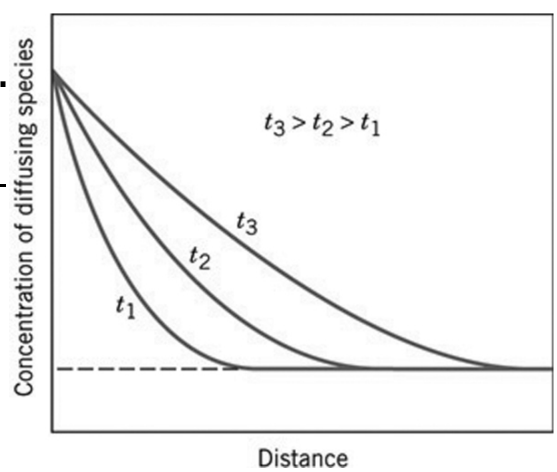


Figure 6.5

Chapter 6 (continued)

Governing Equations of Diffusion (cont.)

nonsteady-state diffusion (cont.)

- **This is described by ______________________**

- **To solve this you need a set of ______________________ .**

Chapter 6 (continued)

nonsteady-state diffusion (cont.)

- **One set of practical boundary conditions consists of a ______ ________ solid with a _____________________ at the surface.**
  - **x = 0 at the surface, and increases into the solid.**
  - **Initially the concentration of the diffusing species is ________________ for all x.**
  - **At time zero the surface concentration is changed to __. This is the instant the diffusion begins.**
  - **The diffusing species never reaches the far side.**

Chapter 6 (continued)

Governing Equations of Diffusion (cont.)

nonsteady-state diffusion (cont.)

- **Mathematically, these boundary conditions look like:**
  - ______________________________
  - ______________________________
  - ______________________________

Chapter 6 (continued)

Governing Equations of Diffusion (cont.)

nonsteady-state diffusion (cont.)

- **This solves to**

where C_x = the concentration at position x
erf is the error function. A tabulated integral.
(see Table 6.1)

- **(see Examples 6.2 and 6.3)**

Chapter 6 (continued)

nonsteady-state diffusion (cont.)

Table 6.1 Tabulation of Error Function Values

z	erf(z)	z	erf(z)	z	erf(z)
0	0	0.55	0.5633	1.3	0.9340
0.025	0.0282	0.60	0.6039	1.4	0.9523
0.05	0.0564	0.65	0.6420	1.5	0.9661
0.10	0.1125	0.70	0.6778	1.6	0.9763
0.15	0.1680	0.75	0.7112	1.7	0.9838
0.20	0.2227	0.80	0.7421	1.8	0.9891
0.25	0.2763	0.85	0.7707	1.9	0.9928
0.30	0.3286	0.90	0.7970	2.0	0.9953
0.35	0.3794	0.95	0.8209	2.2	0.9981
0.40	0.4284	1.0	0.8427	2.4	0.9993
0.45	0.4755	1.1	0.8802	2.6	0.9998
0.50	0.5205	1.2	0.9103	2.8	0.9999

Chapter 6 (continued)

Factors That Influence Diffusion

- **All the factors are seen in the ____________ (Table 6.2)**

Effect of diffusing species

- **Cu in Al vs. Mg in Al**

Effect of crystal structure

- **C in α-Fe vs. C in γ-Fe**

Effect of temperature

- **C in α-Fe at 500°C vs. 900°C (see Figure 6.7)**

Chapter 6 (continued)

Factors That Influence Diffusion (cont.)

Table 6.2 A Tabulation of Diffusion Data

Diffusing Species	*Host Metal*	$D_0(m^2/s)$	*Activation Energy* Q_d *kJ/mol*	*Activation Energy* Q_d *eV/atom*	*Calculated Values* $T(°C)$	*Calculated Values* $D(m^2/s)$
Fe	α-Fe (BCC)	2.8×10^{-4}	251	2.60	500	3.0×10^{-21}
					900	1.8×10^{-15}
Fe	γ-Fe (FCC)	5.0×10^{-5}	284	2.94	900	1.1×10^{-17}
					1100	7.8×10^{-16}
C	α-Fe	6.2×10^{-7}	80	0.83	500	2.4×10^{-12}
					900	1.7×10^{-10}
C	γ-Fe	2.3×10^{-5}	148	1.53	900	5.9×10^{-12}
					1100	5.3×10^{-11}
Cu	Cu	7.8×10^{-5}	211	2.19	500	4.2×10^{-19}
Zn	Cu	2.4×10^{-5}	189	1.96	500	4.0×10^{-18}
Al	Al	2.3×10^{-4}	144	1.49	500	4.2×10^{-14}
Cu	Al	6.5×10^{-5}	136	1.41	500	4.1×10^{-14}
Mg	Al	1.2×10^{-4}	131	1.35	500	1.9×10^{-13}
Cu	Ni	2.7×10^{-5}	256	2.65	500	1.3×10^{-22}

Source: E. A. Brandes and G. B. Brook (Editors), *Smithells Metals Reference Book*, 7th edition, Butterworth-Heinemann, Oxford, 1992.

Chapter 6 (continued)

Factors That Influence Diffusion (cont.)

- **All these effects are seen in Equation 6.8**

where D = the diffusion coefficient

D_0 = a pre-exponential constant

Q_0 = the activation energy (J/mol)

= energy required to get a mole of atoms to diffuse

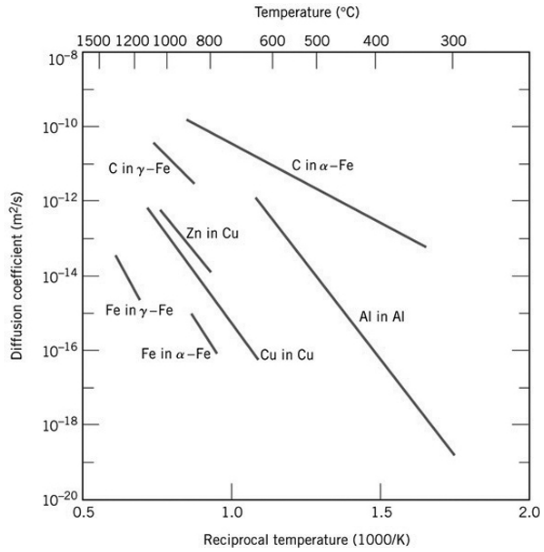
R = the gas constant = 8.314 J/(mol K)

T = the absolute temperature

- **(see Example Problems 6.4 and 6.5)**

Chapter 6 (continued)

Factors That Influence Diffusion (cont.)



Chapter 6 (continued)

Factors That Influence Diffusion (cont.)