

(Isotactic
syndiotactic

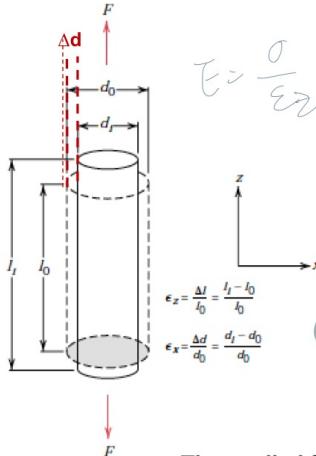
$$\% \text{ Crystallinity} = \frac{\rho_c (\rho_s - \rho_a)}{\rho_s (\rho_c - \rho_a)} \times 100 \%$$

A tensile stress is to be applied along the long axis of a cylindrical brass rod that has a diameter of 10 mm (0.4 in.). Determine the magnitude of the load required to produce a 2.5×10^{-3} mm (10^{-4} in.) change in diameter if the deformation is entirely elastic.

SOLUTION

This deformation situation is represented in the accompanying drawing.

Δd , of 2.5×10^{-3} mm



For the strain in the x direction

$$\epsilon_x = \frac{\Delta d}{d_0} = \frac{-2.5 \times 10^{-3} \text{ mm}}{10 \text{ mm}} = -2.5 \times 10^{-4}$$

$\epsilon = \frac{\Delta d}{d_0} \times V$

For the strain in the z direction

$$\epsilon_z = -\frac{\epsilon_x}{\nu} = -\frac{(-2.5 \times 10^{-4})}{0.34} = 7.35 \times 10^{-4}$$

$\nu = -\frac{\epsilon_x}{\epsilon_z}$

From Table 7-1

$$\sigma = \epsilon_z E = (7.35 \times 10^{-4})(97 \times 10^3 \text{ MPa}) = 71.3 \text{ MPa}$$

The applied force

$$F = \sigma A_0 = \sigma \left(\frac{d_0}{2}\right)^2 \pi$$

$\sigma = \frac{F}{A_0}$

$$= (71.3 \times 10^6 \text{ N/m}^2) \left(\frac{10 \times 10^{-3} \text{ m}}{2}\right)^2 \pi = 5600 \text{ N (1293 lb_f)}$$

Computation of Equilibrium Vacancy Concentration

- Find the equilibrium number of vacancies (N_v) in 1 m^3 of Cu at 1000°C
 - Given:
- | | |
|-----------------------------|--|
| $\rho = 8.4 \text{ g/cm}^3$ | $A_{\text{Cu}} = 63.5 \text{ g/mol}$ |
| $Q_V = 0.9 \text{ eV/atom}$ | $N_A = 6.022 \times 10^{23} \text{ atoms/mol}$ |

$$\frac{A}{\text{mole}} = \rho$$

mole/cm^3

Solution:

1st: Determine the total number of lattice sites N using Equation 4.2

Number of atoms per unit volume for a metal

$$N_{\text{Cu}} = \frac{N_A \rho}{A_{\text{Cu}}} = \frac{(6.022 \times 10^{23} \text{ sites/mol})(8.4 \text{ g/cm}^3)}{63.5 \text{ g/mol}} \left(\frac{10^6 \text{ cm}^3}{\text{m}^3} \right)$$

$$= 8.0 \times 10^{28} \text{ sites/m}^3$$

Ductility and True-stress-at-Fracture Computations

A cylindrical specimen of steel having an original diameter of 12.8 mm (0.505 in.) is tensile tested to fracture and found to have an engineering fracture strength f of 460 MPa (67,000 psi).

If its cross-sectional diameter at fracture is 10.7 mm (0.422 in.), determine:

3/2

(a) The ductility in terms of percent reduction in area.

(a) Ductility is computed using Equation 7.12, as

$$\%RA = \frac{\left(\frac{(12.8 \text{ mm})^2}{2}\pi - \left(\frac{(10.7 \text{ mm})^2}{2}\pi\right)\right)}{\left(\frac{(12.8 \text{ mm})^2}{2}\pi\right)} \times 100$$
$$\%RA = \left(\frac{A_0 - A_f}{A_0}\right) \times 100 = \frac{128.7 \text{ mm}^2 - 89.9 \text{ mm}^2}{128.7 \text{ mm}^2} \times 100 = 30\%$$

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Chapter 7 - 41

(b) The true stress at fracture.

$$F = \sigma_f A_0 = (460 \times 10^6 \text{ N/m}^2)(128.7 \text{ mm}^2) \left(\frac{1 \text{ m}^2}{10^6 \text{ mm}^2}\right) = 59,200 \text{ N}$$

$$\sigma_T = \frac{F}{A_f}$$

Thus, the true stress is calculated as

$$\sigma_T = \frac{F}{A_f} = \frac{59,200 \text{ N}}{(89.9 \text{ mm}^2) \left(\frac{1 \text{ m}^2}{10^6 \text{ mm}^2}\right)}$$
$$= 6.6 \times 10^8 \text{ N/m}^2 = 660 \text{ MPa (95,700 psi)}$$

W. Hume – Rothery rules

- 1. Δr (atomic radius) < 15%
- 2. Proximity in periodic table 元素週期表中的鄰近程度
- i.e., similar electronegativities
- 3. Same crystal structure for pure metals
- 4. Valences 優電子 (價數)
 - All else being equal, a metal will have a greater tendency to dissolve a metal of higher valence than one of lower valence

Chapter 5 - 12

- Solid-state diffusion is mass transport within solid materials by stepwise atomic motion

- Two diffusion mechanisms
 - Vacancy diffusion
 - Interstitial diffusion

- Fick's First Law of Diffusion

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

- Fick's Second Law of Diffusion
 - non-steady state diffusion

$$\frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2}$$

Diffusion 擴散

依原子運動作質量傳遞

Diffusion - Mass transport by atomic motion

- Diffusion Mechanisms

- Gases & Liquids – random (Brownian) motion 隨機布朗運動
- Solids – vacancy diffusion and interstitial diffusion 空位擴散

- Interdiffusion - diffusion of atoms of one material into another material 相互擴散

- Self-diffusion – atomic migration in a pure metal

small. *Atoms*

Deformation of Single Crystals

Example Problem

A single crystal of some metal has a τ_{crss} of 20.7 MPa and is exposed to a tensile stress of 45 MPa.

- (a) Will yielding occur when $\phi = 60^\circ$ and $\lambda = 35^\circ$?
- (b) If not, what stress is necessary?

Solution:

(a) First calculate τ_R

$$\tau_R = \sigma \cos \lambda \cos \phi$$

$$\tau_R = (45 \text{ MPa}) [\cos(35^\circ) \cos(60^\circ)]$$

$$= 18.4 \text{ MPa}$$

Since τ_R (18.4 MPa) < τ_{crss} (20.7 MPa) -- no yielding

Deformation of Single Crystals

Example Problem (cont.)

(b) To calculate the required tensile stress to cause yielding use the equation:

$$\sigma_y = \frac{\tau_{\text{crss}}}{\cos \lambda \cos \phi}$$

With specified values

$$\begin{aligned}\sigma_y &= \frac{20.7 \text{ MPa}}{\cos(35^\circ) \cos(60^\circ)} \\ &= 50.5 \text{ MPa}\end{aligned}$$

Therefore, to cause yielding,

$$\sigma \geq 50.5 \text{ MPa}$$

(b) To calculate the required tensile stress to cause yielding use the equation:

$$\sigma_y = \frac{\tau_{\text{crss}}}{\cos \lambda \cos \phi}$$

With specified values

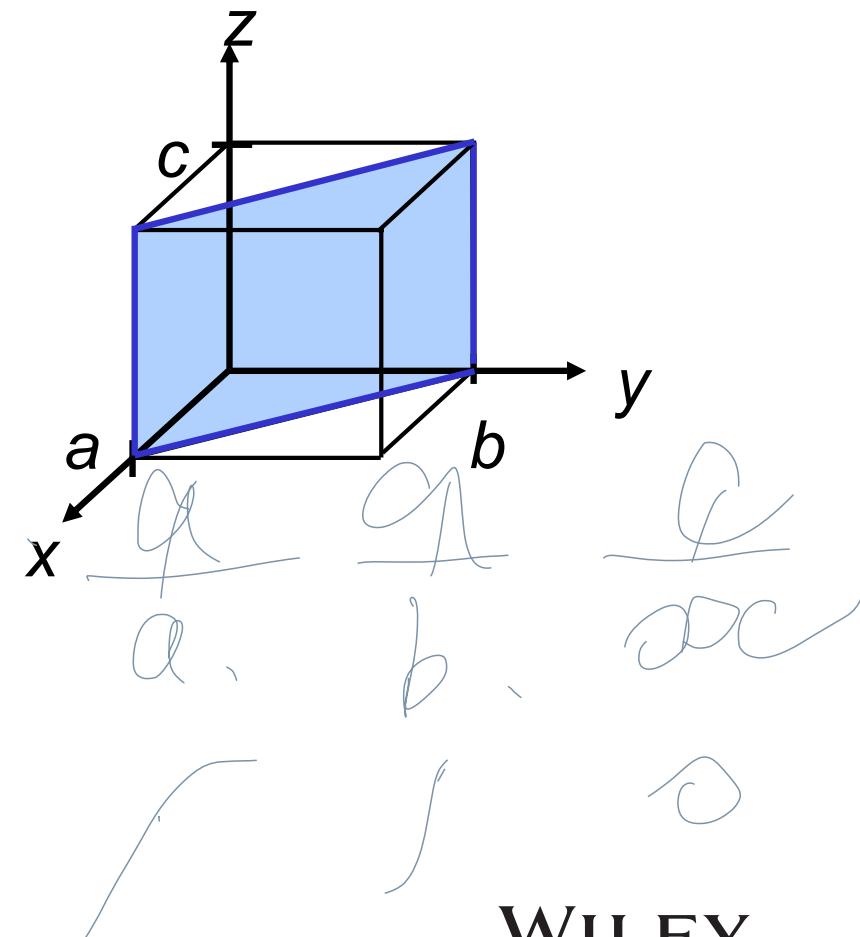
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Therefore, to cause yielding, $\sigma \geq 50.5 \text{ MPa}$

Crystallographic Planes

Example Problem I

	x	y	z
1. Relocate origin – not needed			
2. Intercepts	a	b	∞c
3. Reciprocals	$1/a$	$1/b$	$1/\infty c$
4. Normalize	a/a	b/b	$c/\infty c$
	1	1	0
5. Reduction	1	1	0
6. Miller Indices	(110)		

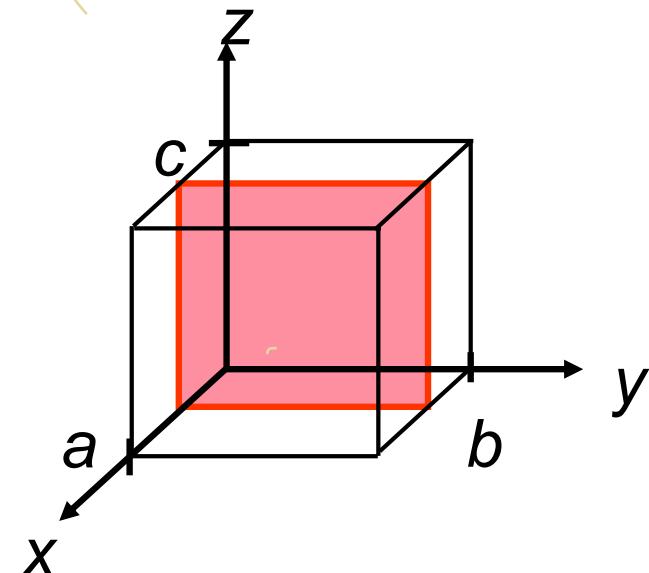


Crystallographic Planes

Example Problem II

	x	y	z
1. Relocate origin – not needed			
2. Intercepts	$a/2$	∞b	∞c
3. Reciprocals	$2/a$	$1/\infty b$	$1/\infty c$
4. Normalize	$2a/a$	$b/\infty b$	$c/\infty c$
	2	0	0
5. Reduction	2	0	0
6. Miller Indices	(200)		

$(\frac{1}{2}a, \infty b, \infty c)$



$\frac{1}{2}a$

∞b ∞c

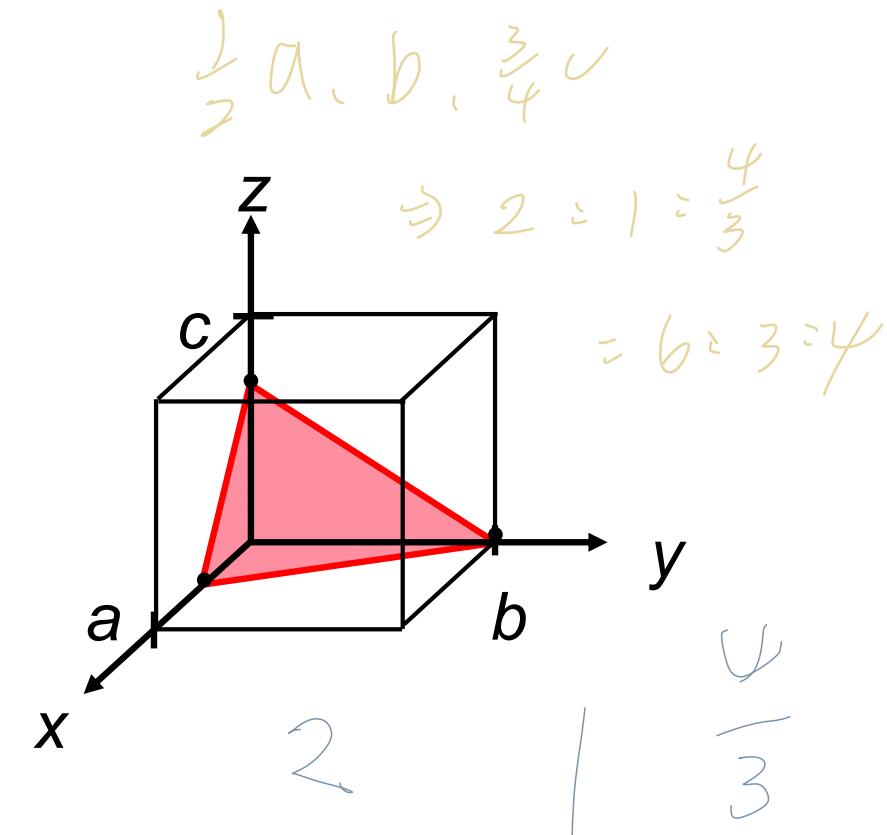
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Crystallographic Planes

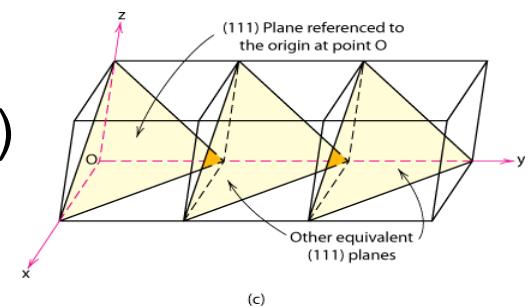
Example Problem III

- | | x | y | z |
|---------------------------------|--------|-------|---------|
| 1. Relocate origin – not needed | | | |
| 2. Intercepts | $a/2$ | b | $3c/4$ |
| 3. Reciprocals | $2/a$ | $1/b$ | $4/3c$ |
| 4. Normalize | $2a/a$ | b/b | $4c/3c$ |
| | 2 | 1 | $4/3$ |
| 5. Reduction (x3) | 6 | 3 | 4 |
| 6. Miller Indices | (634) | | |



Family of planes – all planes that are crystallographically equivalent (have the same atomic packing) – indicated by indices in **braces**

Ex: **{100}** = (100), (010), (001), ($\bar{1}00$), (0 $\bar{1}0$), (00 $\bar{1}$)

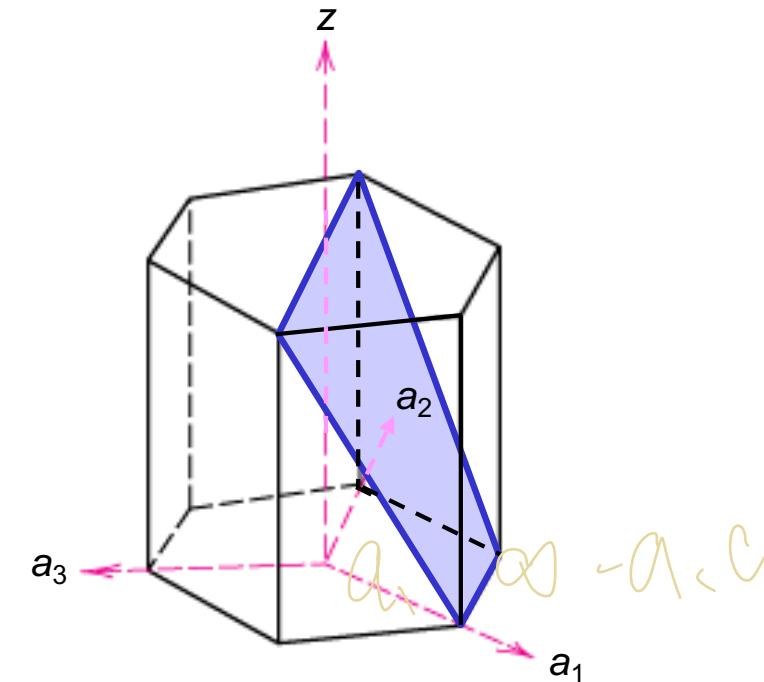


Crystallographic Planes (HCP)

- For **hexagonal unit cells** a similar procedure is used
 - Determine the intercepts with the a_1 , a_2 , and z axes, then determine the **Miller-Bravais Indices h , k , i , and l**

example

	a_1	a_2	a_3	c
1. Relocate origin – not needed				
2. Intercepts	a	∞	$-a$	c
3. Reciprocals	$1/a$	$1/\infty$	$-1/a$	$1/c$
4. Normalize	a/a	a/∞	$-a/a$	c/c
5. Reduction	1	0	-1	1
6. Miller-Bravais Indices	$(10\bar{1}1)$			



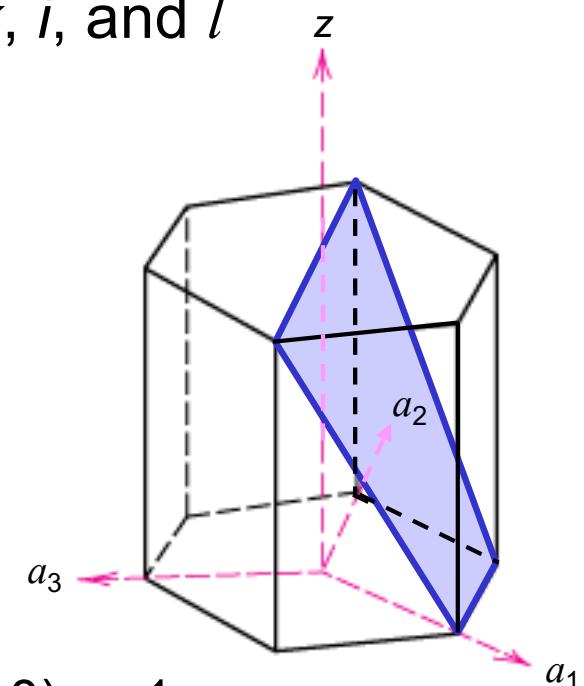
Crystallographic Planes (HCP)

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example

$a_1 \quad a_2 \quad c$

1. Relocate origin – not needed
2. Intercepts $a \quad \infty a \quad c$
3. Reciprocals $1/a \quad 1/\infty a \quad 1/c$
4. Normalize $a/a \quad a/\infty a \quad c/c$
 $1 \quad 0 \quad 1$
5. Reduction $h = 1 \quad k = 0 \quad l = 1$
6. Determine index $i = -(h + k) \quad i = -(1 + 0) = -1$
7. Miller-Bravais Indices $(10\bar{1}1)$



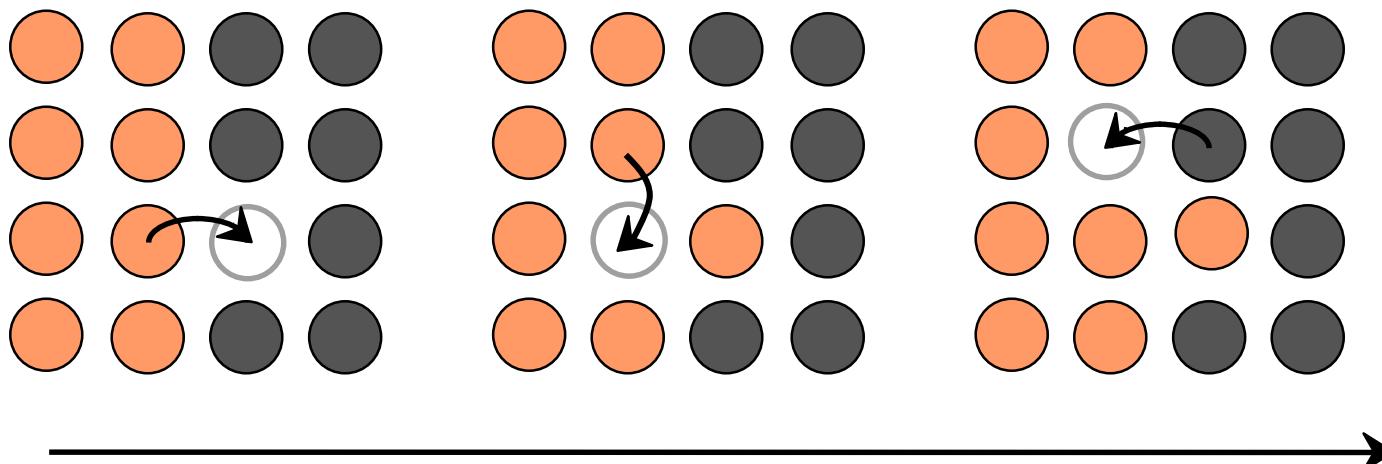
Diffusion Mechanism I

空缺擴散
間隙擴散

Vacancy Diffusion

原子和空缺的交互作用

- atoms and vacancies exchange positions
- applies to host and substitutional impurity atoms
- diffusion rate depends on:
 - number of vacancies 空缺
 - activation energy to exchange. 活化能



Influence of Temperature on Diffusion

- Diffusion coefficient increases with increasing T

$$D \propto \frac{1}{T}$$
$$D = D_o \exp\left(-\frac{Q_d}{RT}\right)$$

(活化能)
取決於物質的特性，也是 T 的修正項
 D_o constant
T 的修正項
氣體常數



D = diffusion coefficient [m^2/s]

D_o = pre-exponential [m^2/s]

Q_d = activation energy [J/mol]

R = gas constant [8.314 J/mol-K]

T = absolute temperature [K]

Non-steady State Diffusion (cont.)

$$\frac{dC}{dt} = D \frac{d^2C}{dx^2}$$

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

$C(x,t)$ = Conc. at point x at time t

$\operatorname{erf}(z)$ = error function

z and $\operatorname{erf}(z)$ values are given in Table

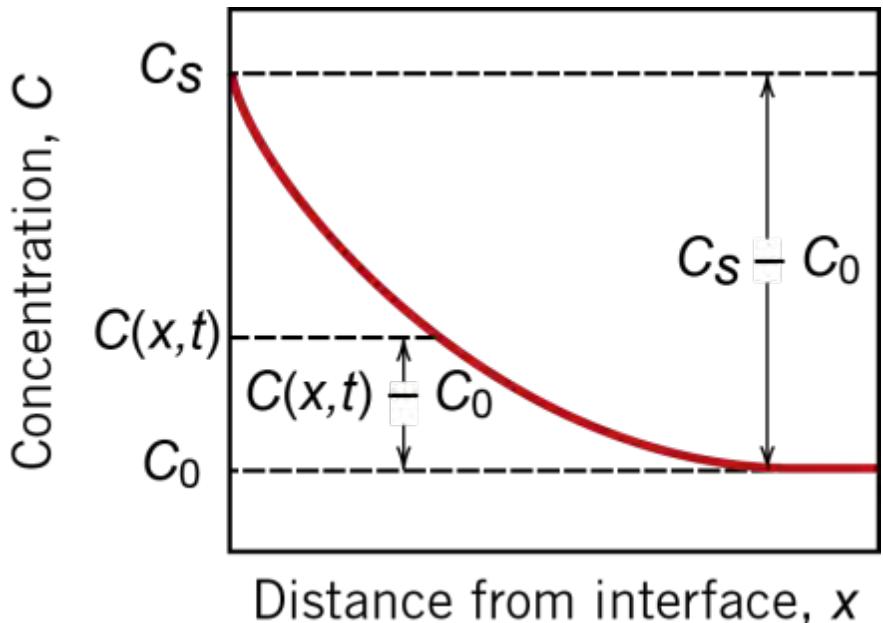


Fig. 6.6, Callister & Rethwisch 5e.

Example Problem (cont.):

Solution: use Eqn. 5.5

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

Data for problem tabulated as follows:

- $t = 49.5$ h
- $C_x = 0.35$ wt%
- $C_o = 0.20$ wt%

$$x = 4 \times 10^{-3} \text{ m}$$

$$C_s = 1.0 \text{ wt\%}$$

$$\frac{C(x,t) - C_o}{C_s - C_o} = \frac{0.35 - 0.20}{1.0 - 0.20} = 1 - \operatorname{erf}\left(\frac{x}{2\sqrt{Dt}}\right) = 1 - \operatorname{erf}(z)$$

$$\operatorname{erf}(z) = 0.8125$$

Example Problem (cont.):

We must now determine from Table 5.1 the value of z for which the error function is 0.8125. An interpolation is necessary as follows

z	$\text{erf}(z)$
0.90	0.7970
z	0.8125
0.95	0.8209

$$\frac{z - 0.90}{0.95 - 0.90} = \frac{0.8125 - 0.7970}{0.8209 - 0.7970}$$
$$z = 0.93$$

Now solve for D

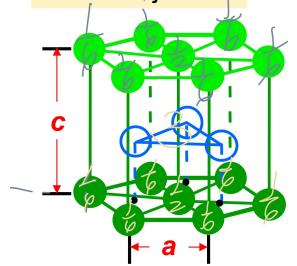
$$z = \frac{x}{2\sqrt{Dt}} \longrightarrow D = \frac{x^2}{4z^2 t}$$

$$\therefore D = \left(\frac{x^2}{4z^2 t} \right) = \frac{(4 \times 10^{-3} \text{ m})^2}{(4)(0.93)^2 (49.5 \text{ h})} \frac{1 \text{ h}}{3600 \text{ s}} = 2.6 \times 10^{-11} \text{ m}^2/\text{s}$$

Example Problem (cont.):

- To solve for the temperature at which D has the above value, we use a rearranged form of Equation

}



$$T = \frac{Q_d}{R(\ln D_o - \ln D)}$$

As known, (Table), for diffusion of C in FCC Fe

$$D_o = 2.3 \times 10^{-5} \text{ m}^2/\text{s}$$

$$Q_d = 148,000 \text{ J/mol}$$

$$T = \frac{148,000 \text{ J/mol}}{(8.314 \text{ J/mol-K})[\ln (2.3 \times 10^{-5} \text{ m}^2/\text{s}) - \ln (2.6 \times 10^{-11} \text{ m}^2/\text{s})]}$$

$$T = 1300 \text{ K} = 1027^\circ \text{ C}$$

$$D = D_o \exp -\frac{Q_d}{RT}$$

D = diffusion coefficient [m^2/s]

D_o = pre-exponential [m^2/s]

Q_d = activation energy [J/mol]

R = gas constant [8.314 J/mol-K]

T = absolute temperature [K]

Computations of the Density and Percent Crystallinity of Polyethylene

(b) Calculate the % crystallinity of PE

(✓) $\rho_c = 0.998 \text{ g/cm}^3$

(✗) $\rho_a = 0.870 \text{ g/cm}^3$

$\rho_s = 0.925 \text{ g/cm}^3$

$$\% \text{ crystallinity} = \frac{\rho_c(\rho_s - \rho_a)}{\rho_s(\rho_c - \rho_a)} \times 100$$

$$\begin{aligned}\% \text{ Crystallinity} &= \frac{0.998 (0.925 - 0.870)}{0.925 (0.998 - 0.870)} \times 100 \\ &= 46.4\%\end{aligned}$$

The Rubbery state

- Amorphous
- Random coils have enough thermal energy for rotation to occur around single bonds.
- When melting, each random coil is continuously changing shape.
- Soft, flexible and extensible, due to the molecular motion available to the molecules.

The Glassy state

- Temperature drops, the rate of rotation around main chain bonds becomes slower and the chain gets stiffer.
- At a low enough temperature, single bond rotation ceases and the interpenetrated random coils become frozen in space. (the glassy state)
- The temperature where single bond rotation ceases is called the glass transition temperature (T_g)
- $< T_g$, hard, stiff and brittle.