

2019 Fall

Introduction to Materials Science and Engineering

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Contents for previous class

Chapter 6: Imperfections in Solids

I. Point defects

- Point defects in metals/ceramics/polymers, impurities in solids

II. Dislocations-Linear defects

- Edge/ Screw/ Mix dislocation

III. Interfacial defects

- External surfaces/ Grain boundaries/ Phase boundaries (stacking fault)/ Twin boundaries/ domain boundaries

IV. Bulk or Volume defects

- pores/ cracks/ foreign inclusions, and other phases

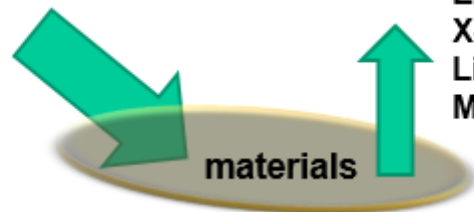
V. Microscopic Examination

- Basic concepts of microscopy
- Microscopic techniques : Optical microscopy (Grain-size determination)
/ Electron microscopy/ Scanning probe microscopy

Chapter 6: Imperfections in Solids

- Point, Line, Area and Volume defects exist in solids.
- The number and type of defects can be varied and controlled (e.g., temperature controls vacancy concentration).
- Defects affect material properties (e.g., grain boundaries control crystal slip).
- Defects may be desirable or undesirable (e.g., dislocations may be good or bad, depending on whether plastic deformation is desirable or not).
- Observation of Microstructure: to make image from the collection of defects in the materials

Electron
X-ray
Laser
Light
Shockwave
Mechanical



Electron
X-ray
Light
Mechanical



OM, SEM, TEM, EXAFS, AFM, SPM

Contents for today's class

Chapter 7: Diffusion

I. Introduction of diffusion

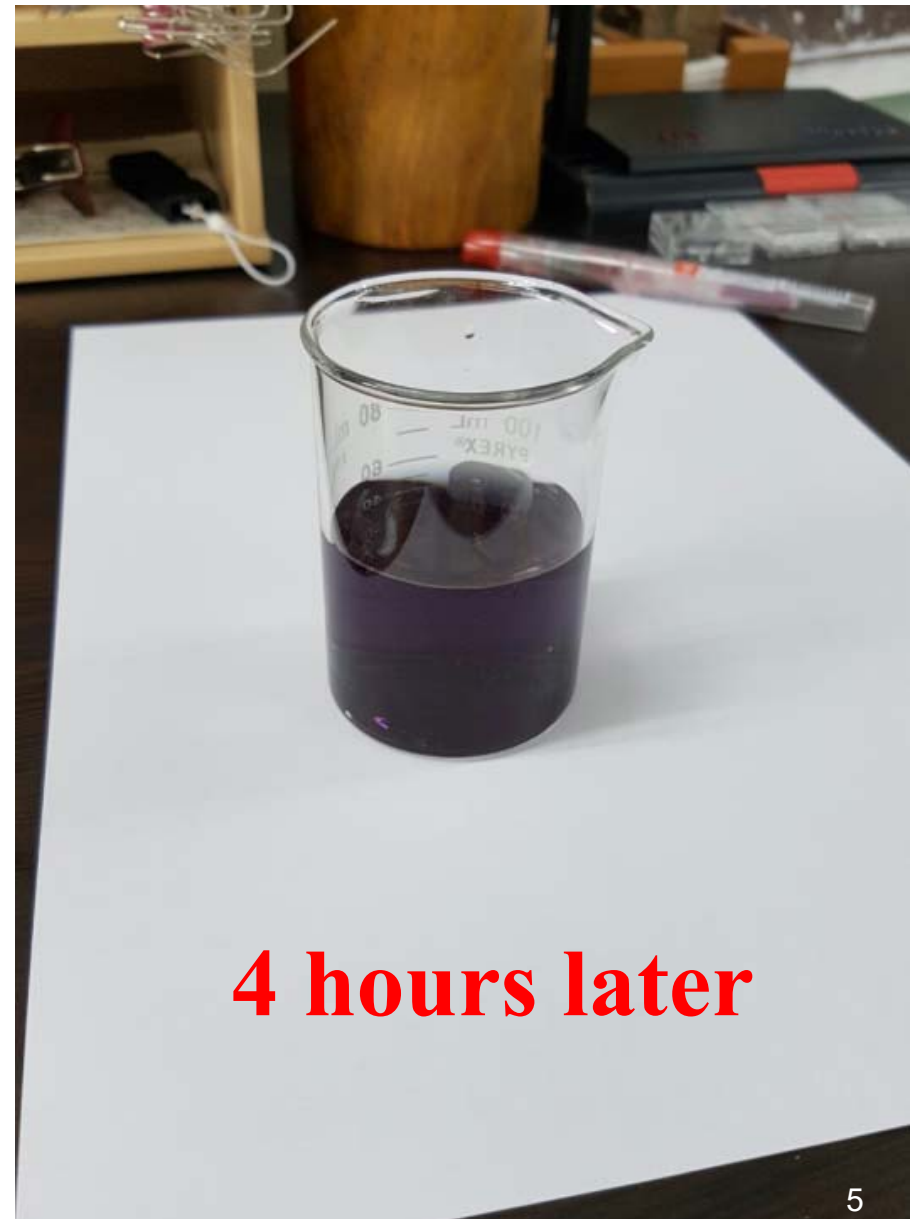
II. Diffusion mechanisms

III. Steady-state diffusion

IV. Nonsteady-state diffusion

V. Factors that influences diffusion

Ink dropped in the water



1. Introduction of Diffusion

- atoms and molecules can be quite mobile in both liquids and solids, especially at high temp
 - Drop of ink in a beaker of water → spread, water evenly colored
 - **Intermixing at molecular level → diffusion**
- continuous motion of H₂O molecules in water at R.T. → **self-diffusion**
- atomic-scale motion (diffusion) **in liquids** is relatively rapid and easily to visualize
- more difficult to visualize diffusion **in rigid solids**, but it does occur

Diffusion

- **Diffusion: Mass transport by atomic motion**
- Heat treatments alter the properties of materials

Only possible by
atom movement



Internal structure of
material must change

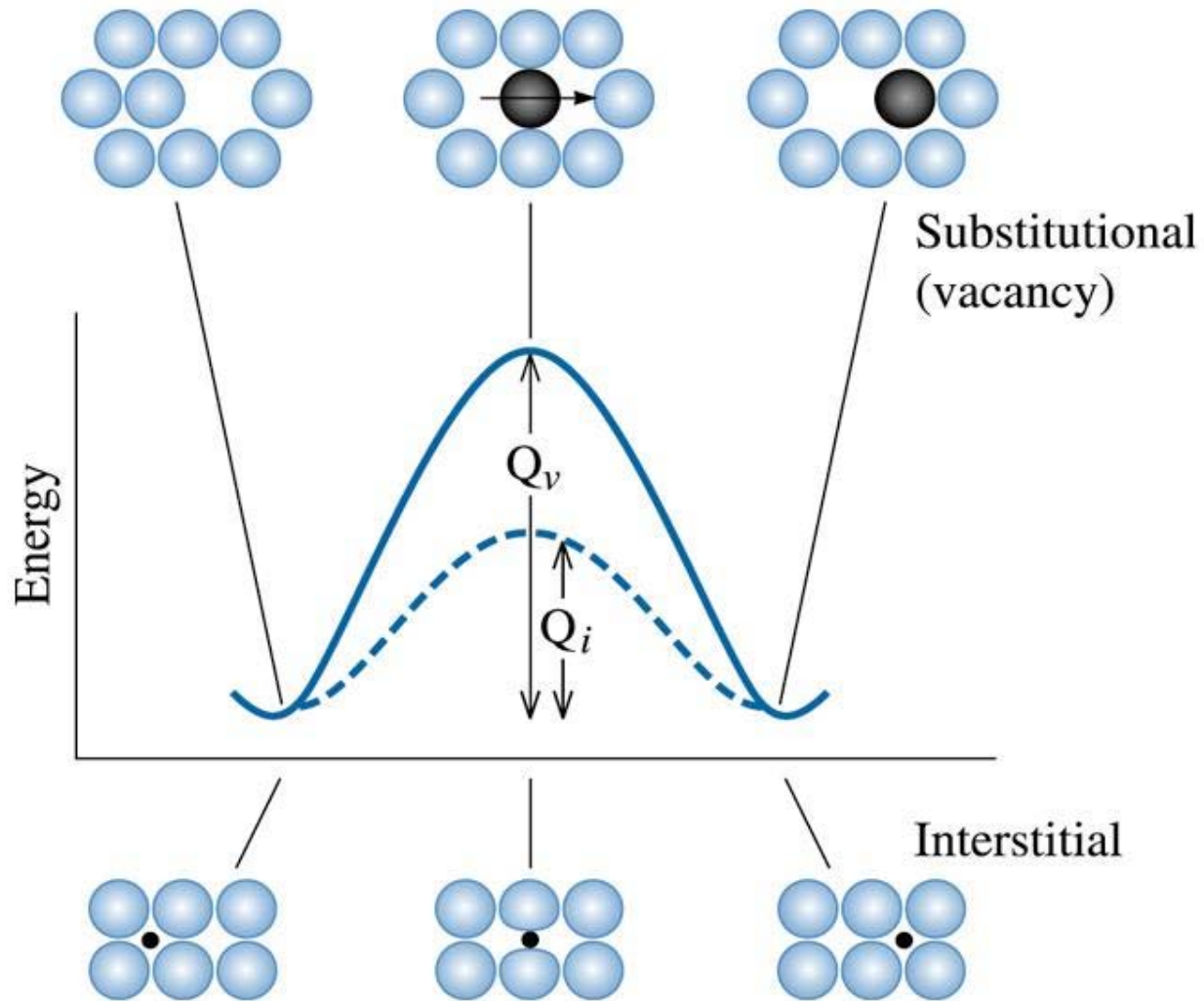


- Diffusion required for:
 - Heat treatment of metals, Ceramics sintering, Solidification, Integrated circuits, and solar cells
 - Electrical conductivity of ceramic materials
- Mechanisms
 - Gases & Liquids – random (Brownian) motion
 - Solids – vacancy diffusion or interstitial diffusion

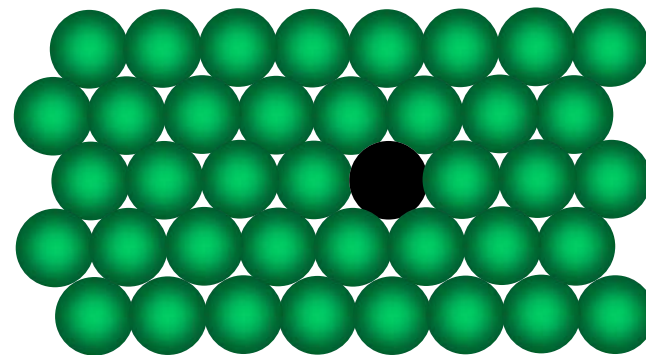
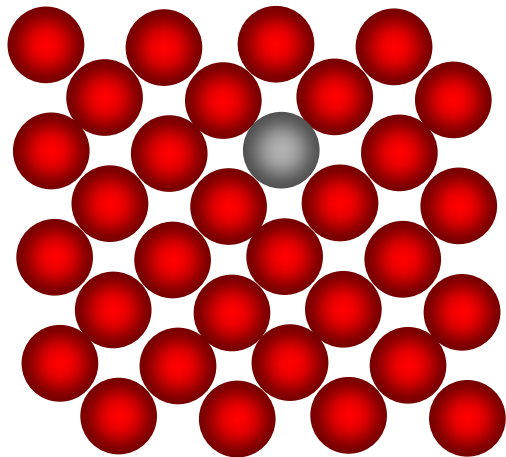
Diffusion Concepts

- reactions in solid state occur by spontaneous rearrangement of atoms into a more stable state
- for reactions to proceed from an unreacted to a reacted state, atoms must have enough energy to overcome an activation energy barrier

Diffusion Concepts



Diffusion



2. Diffusion mechanism

- Tendency to be random
 - Entropy term in the total energy $\uparrow \rightarrow$ Chemical Potential \downarrow
- From higher concentration to lower concentration
 - few exceptions, but take it granted for now.

I. Vacancy diffusion

(a) Self-diffusion

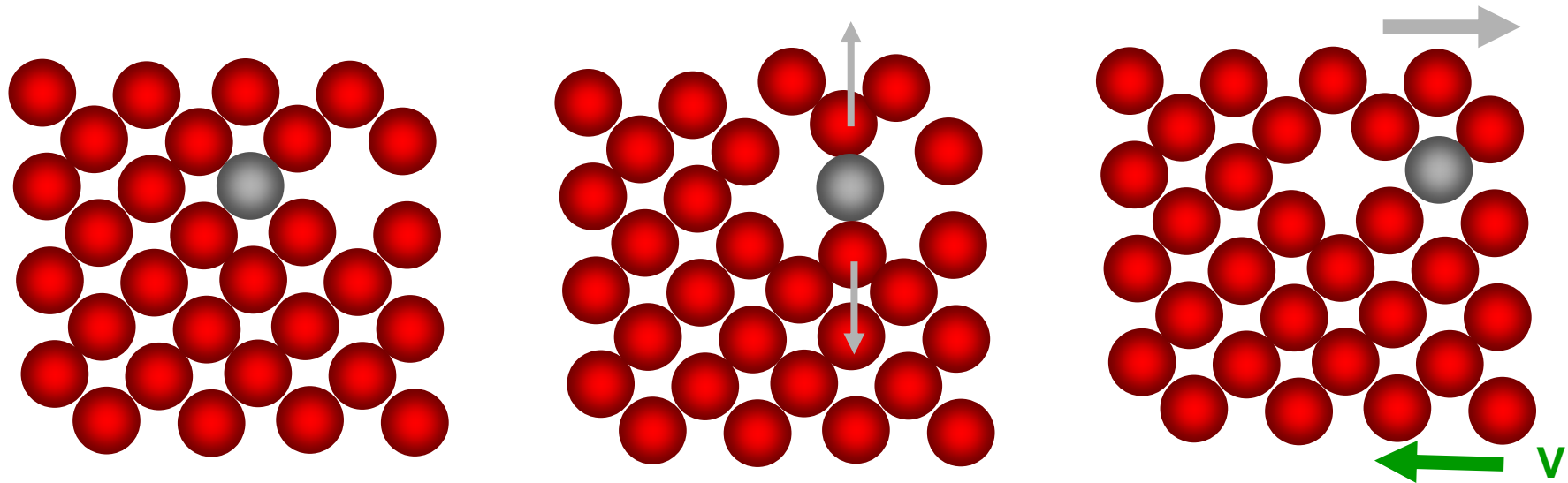
(b) Interdiffusion

II. Interstitial diffusion

I. Vacancy Diffusion

- What is needed to make solid-state diffusion happen?

→ **POINT DEFECTS**



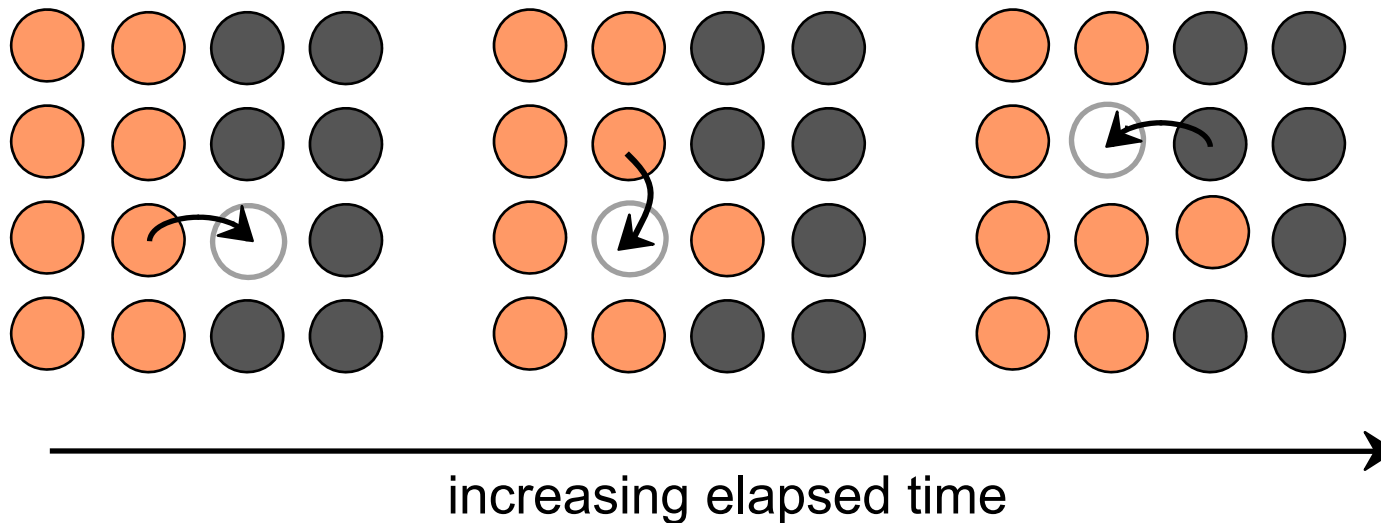
I. Vacancy Diffusion

- **atom interchange** from a normal lattice position to an adjacent vacant lattice site
- the extent of vacancy diffusion is controlled by the concentration of these defects
- the direction of vacancy motion is opposite to direction of diffusing atoms
- both (a) **self-diffusion** and (b) **interdiffusion** occur by this mechanism

Diffusion Mechanisms

Vacancy Diffusion:

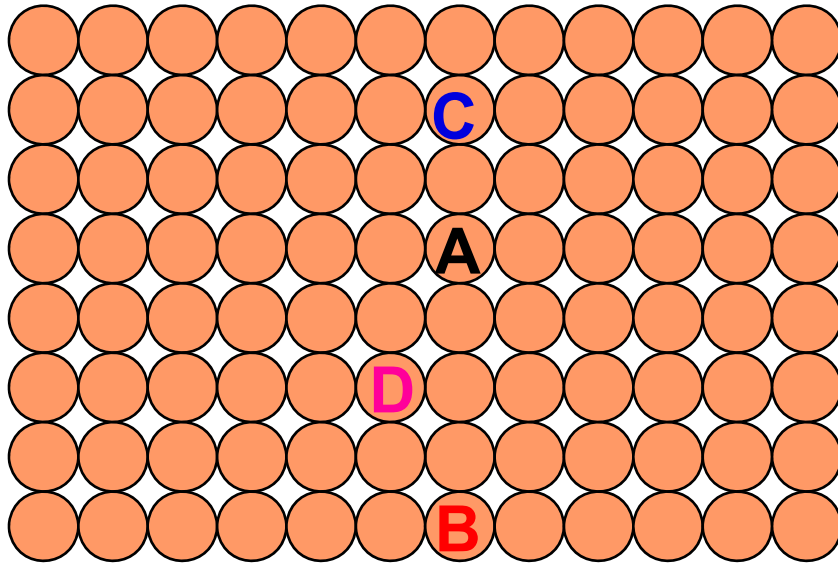
- atoms exchange with vacancies
- applies to **substitutional impurities atoms**
- rate depends on:
 - number of vacancies
 - activation energy to exchange.



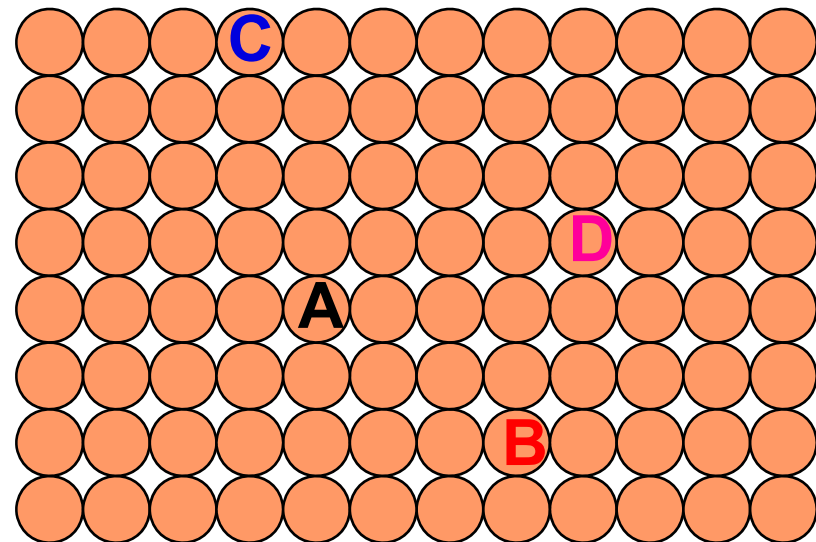
I-(a) Self-Diffusion

- **Self-diffusion:** In an elemental solid, atoms also migrate

Label some atoms

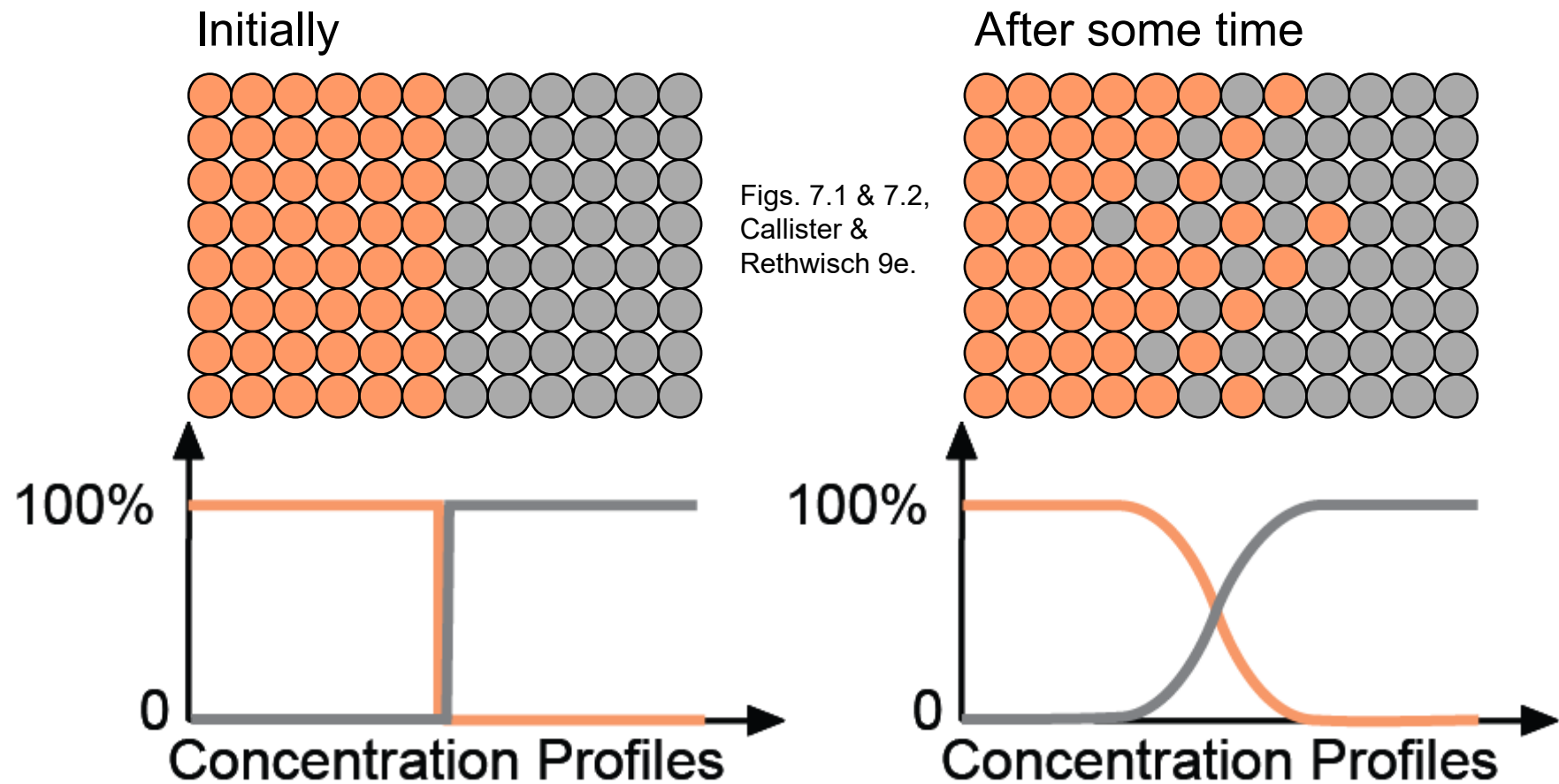


After some time



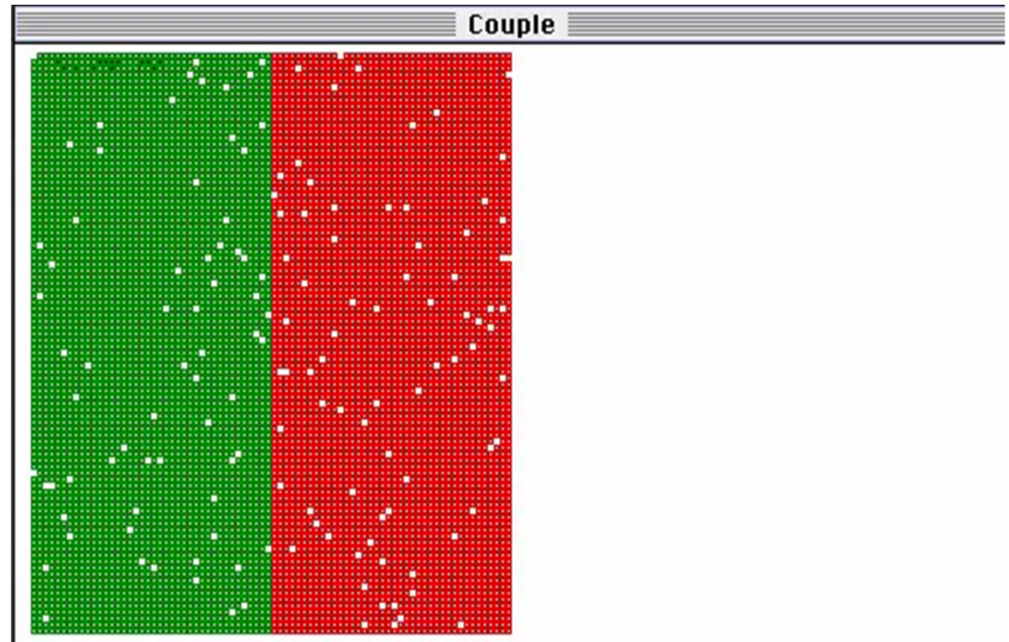
I-(b) Interdiffusion

- **Interdiffusion:** In an alloy, atoms tend to migrate from regions of high conc. to regions of low conc.

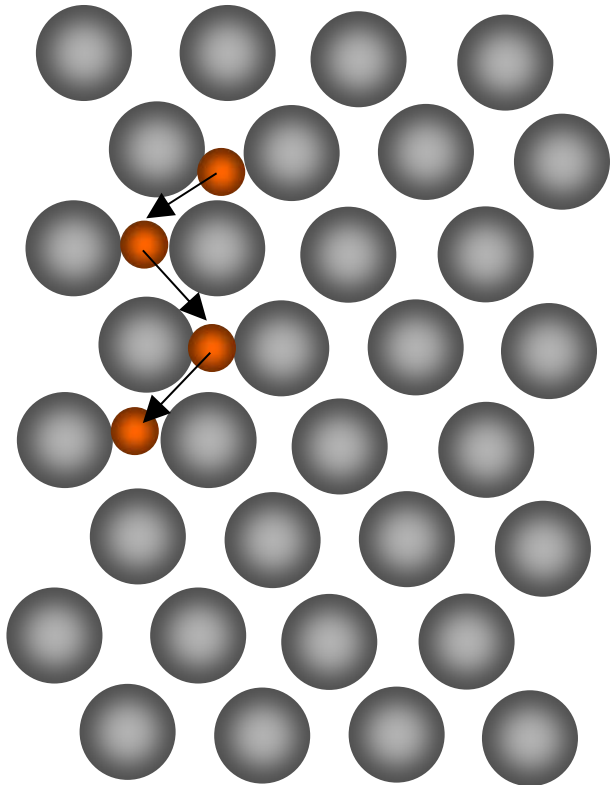


Diffusion Simulation

- Simulation of inter-diffusion across an interface
- Rate of substitutional diffusion depends on
 - **vacancy concentration**
 - **frequency of jumping**



II. Interstitial Diffusion



- migration of interstitial atoms from an interstitial position to adjacent empty one.
- Typical interstitial atoms:
hydrogen, carbon, nitrogen, and oxygen.
- in most metals, interstitial diffusion occurs **much more rapidly** than vacancy diffusion.

Processing Using Diffusion (1)

- Case Hardening:
 - Diffuse carbon atoms into the host iron atoms at the surface
 - Example of interstitial diffusion is a case hardened gear

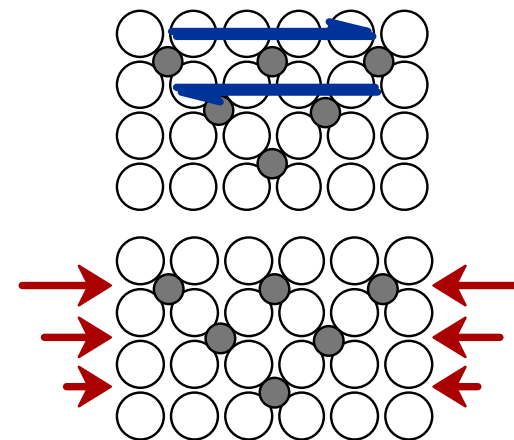


Chapter-opening photograph, Chapter 7, Callister & Rethwisch 9e. (Courtesy of Surface Division, Midland-Ross.)

- Result: The presence of C atoms makes iron (steel) harder.

The "Case" is

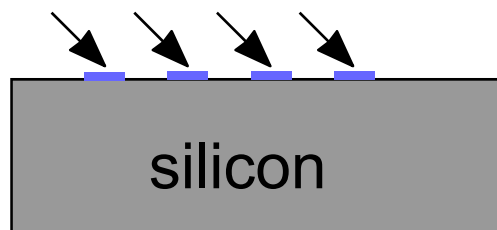
- hard to deform: C atoms "lock" planes from **shearing**
- hard to crack: C atoms put the surface in **compression**



Processing Using Diffusion (2)

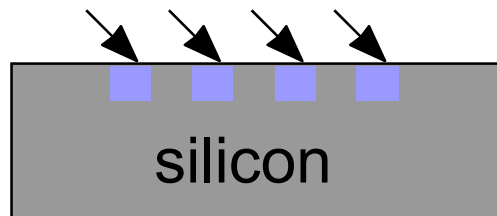
- **Doping** silicon with phosphorus for n-type semiconductors:
- Process:

1. Deposit **P** rich layers on surface.

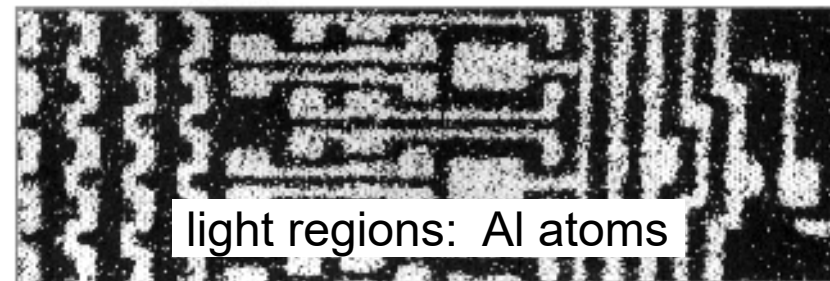
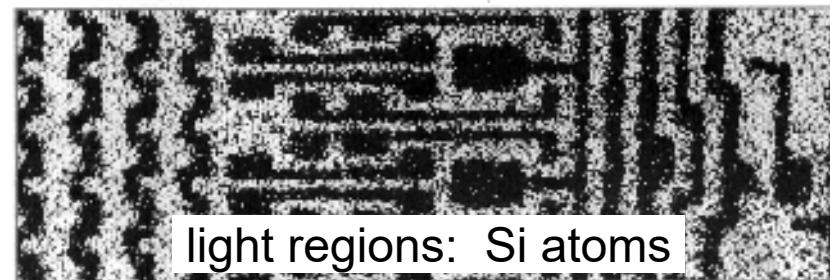
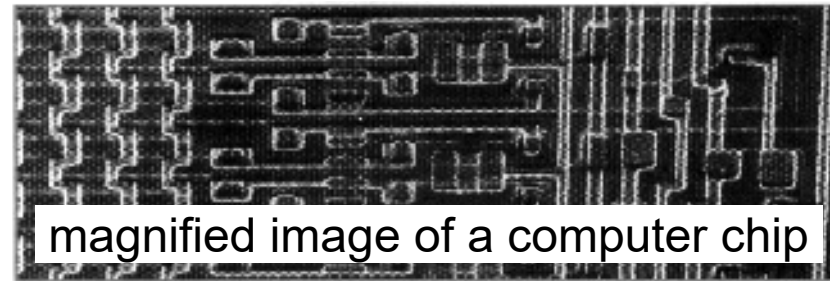


2. Heat it.

3. Result: Doped semiconductor regions.



← 0.5 mm →



Adapted from Figure 19.27, Callister & Rethwisch 9e.

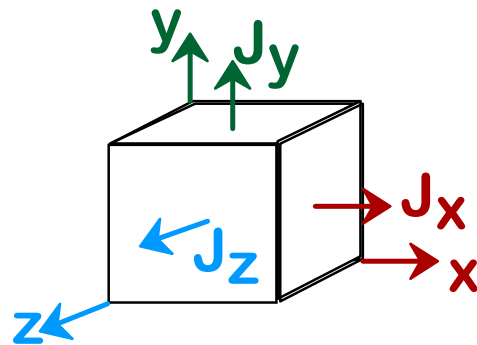
Diffusion

- How do we quantify the amount or rate of diffusion?

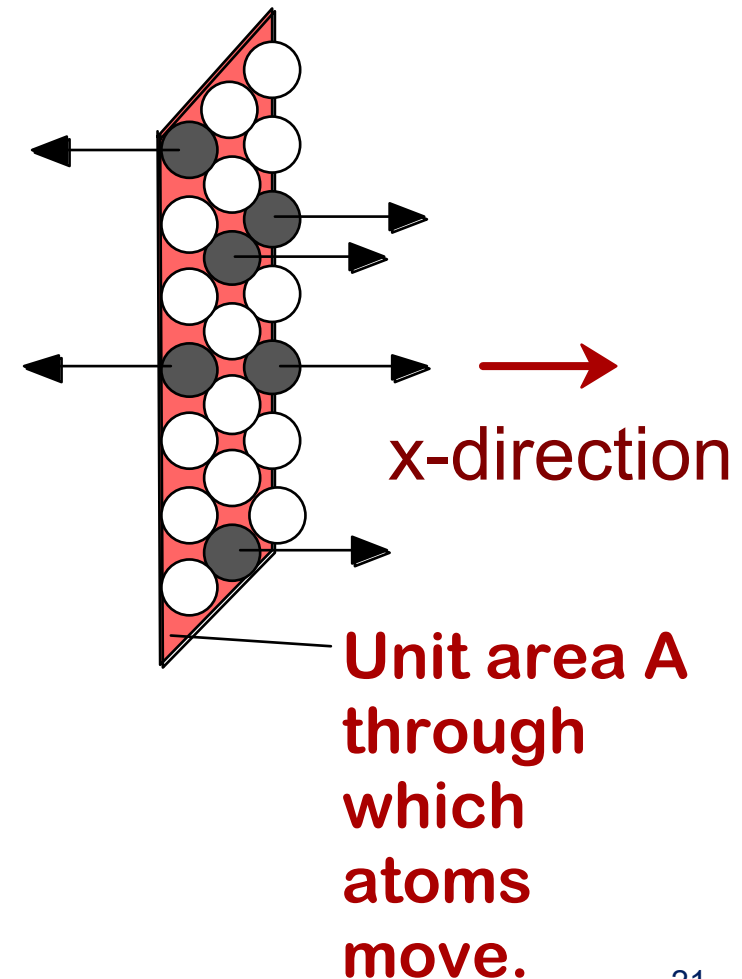
- **Flux:** # of atoms passing through a plane of unit area per unit time

$$J = \frac{1}{A} \frac{dM}{dt} \Rightarrow \left[\frac{\text{kg}}{\text{m}^2\text{s}} \right] \text{ or } \left[\frac{\text{atoms}}{\text{m}^2\text{s}} \right]$$

- Directional Quantity



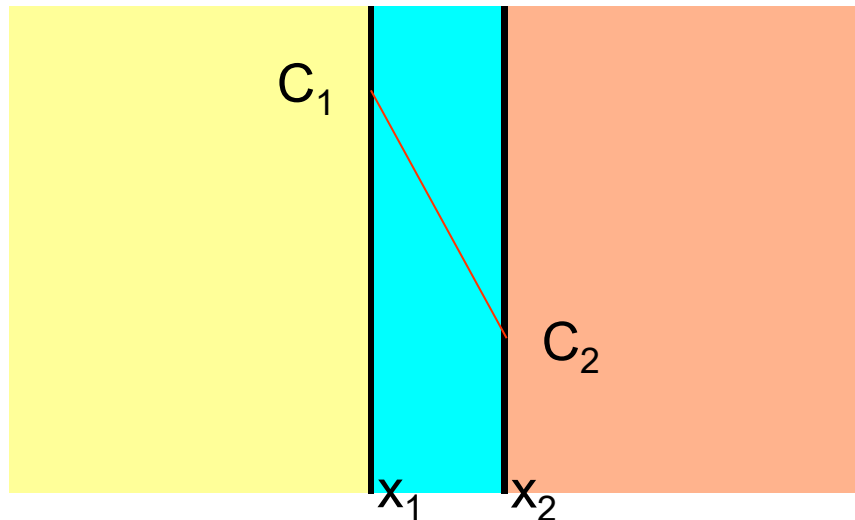
- Flux can be measured for:
 - vacancies
 - host (A) atoms
 - impurity (B) atoms



3-1. Steady-State Diffusion

Rate of diffusion independent of time

Flux proportional to concentration gradient = $\frac{dC}{dx}$



Fick's first law of diffusion

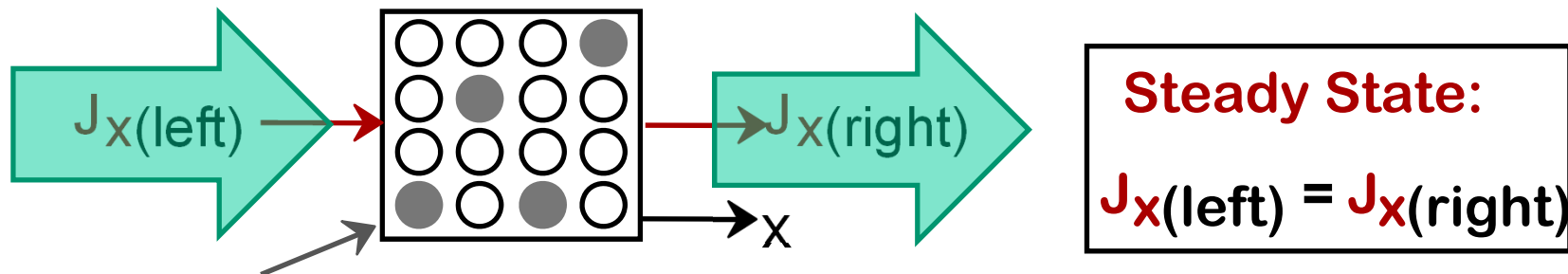
$$J = -D \frac{dC}{dx}$$

$D \equiv$ diffusion coefficient

if linear $\frac{dC}{dx} \cong \frac{\Delta C}{\Delta x} = \frac{C_2 - C_1}{x_2 - x_1}$

Steady State Diffusion - Fick's 1st law

- **Steady State:** the concentration profile doesn't change with time



- Apply Fick's First Law

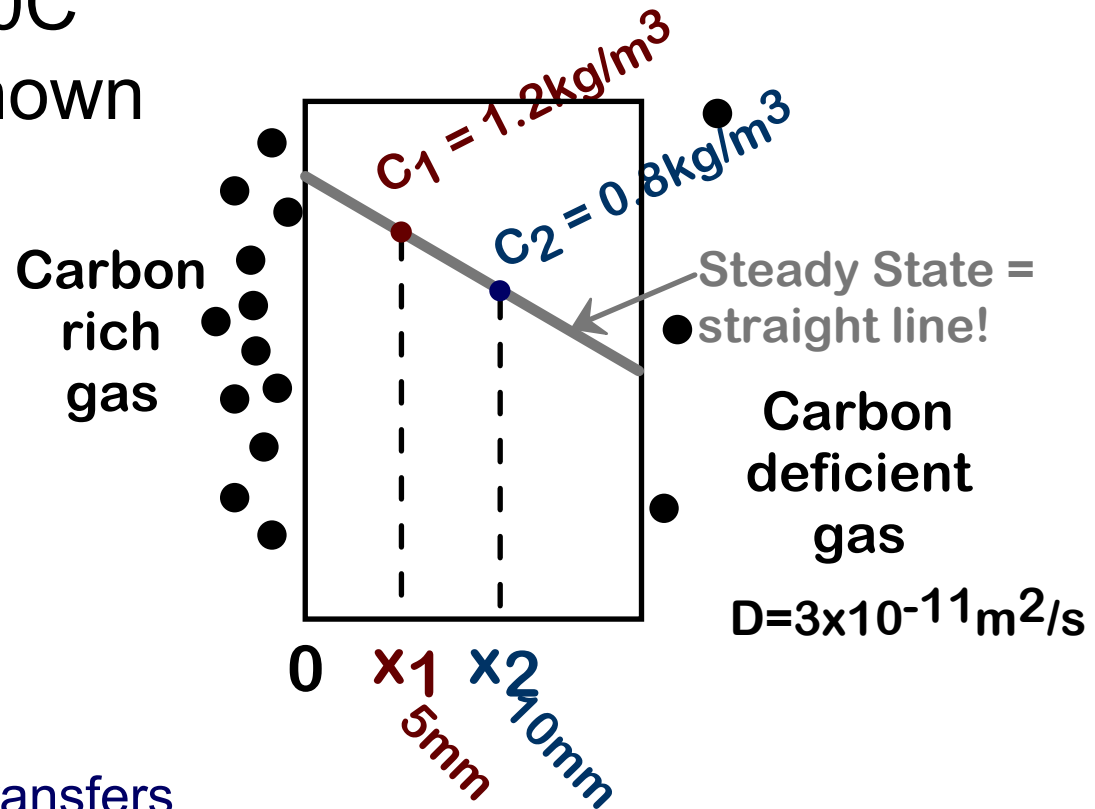
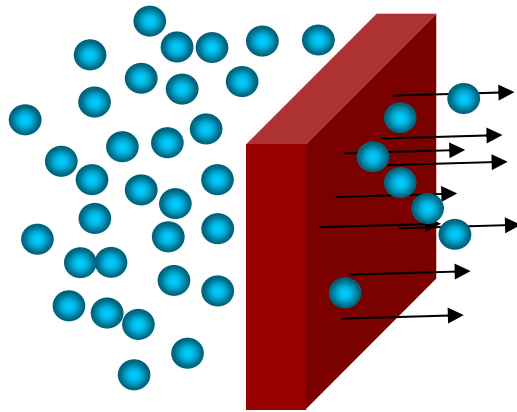
$$J_x = -D \frac{dC}{dx}$$

- If $J_x(\text{left}) = J_x(\text{right})$, then $\left(\frac{dC}{dx}\right)_{\text{left}} = \left(\frac{dC}{dx}\right)_{\text{right}}$

- Result: the slope, dC/dx , must be constant (i.e., slope doesn't vary with position as well as time)!

Example I: Steady State Diffusion

- Steel plate at 700C with geometry shown



- Q: How much carbon transfers from the rich to the deficient side?

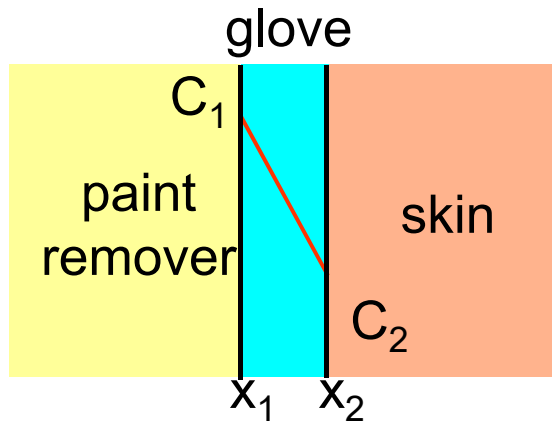
$$J = -D \frac{C_2 - C_1}{x_2 - x_1} = 2.4 \times 10^{-9} \frac{\text{kg}}{\text{m}^2 \text{s}}$$

Example II: Chemical Protective Clothing (CPC)

- Methylene chloride is a common ingredient of paint removers. Besides being an irritant, it also may be absorbed through skin. When using this paint remover, protective gloves should be worn.
- If butyl rubber gloves (0.04 cm thick) are used, what is the diffusive flux of methylene chloride through the glove?
- Data:
 - diffusion coefficient in butyl rubber:
 $D = 110 \times 10^{-8} \text{ cm}^2/\text{s}$
 - surface concentrations:
 $C_1 = 0.44 \text{ g/cm}^3$
 $C_2 = 0.02 \text{ g/cm}^3$

Example (cont).

- **Solution** – assuming linear conc. gradient



$$J = -D \frac{dC}{dx} \cong -D \frac{C_2 - C_1}{x_2 - x_1}$$

Data: $D = 110 \times 10^{-8} \text{ cm}^2/\text{s}$

$$C_1 = 0.44 \text{ g/cm}^3$$

$$C_2 = 0.02 \text{ g/cm}^3$$

$$x_2 - x_1 = 0.04 \text{ cm}$$

$$J = -(110 \times 10^{-8} \text{ cm}^2/\text{s}) \frac{(0.02 \text{ g/cm}^3 - 0.44 \text{ g/cm}^3)}{(0.04 \text{ cm})} = 1.16 \times 10^{-5} \frac{\text{g}}{\text{cm}^2\text{s}}$$

3-II. Non-steady State Diffusion

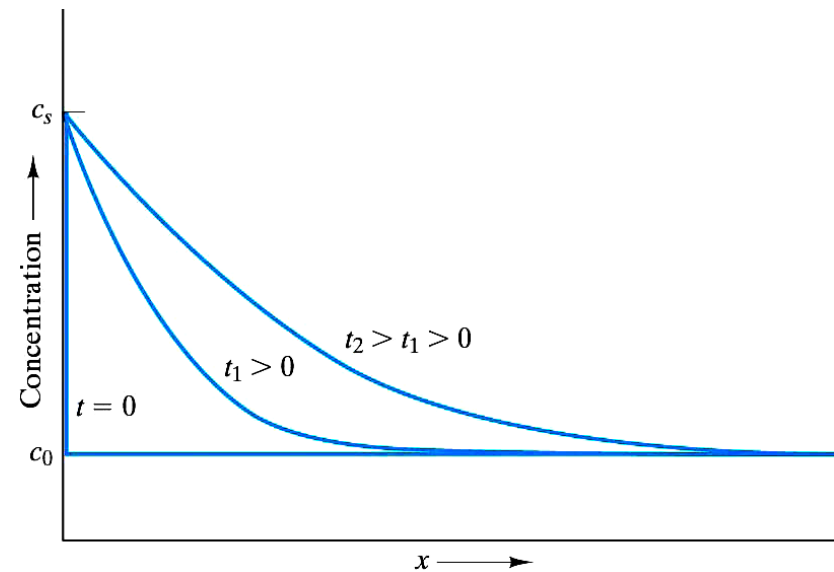
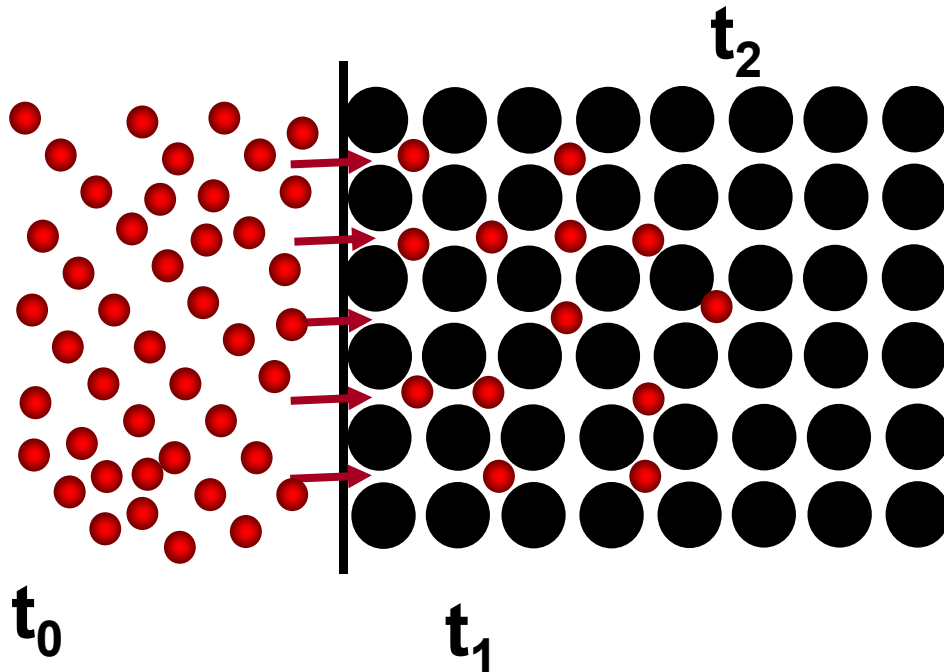
- The concentration of diffusing species is a function of both time and position $C = C(x,t)$
- In this case **Fick's Second Law** is used

Fick's Second Law

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

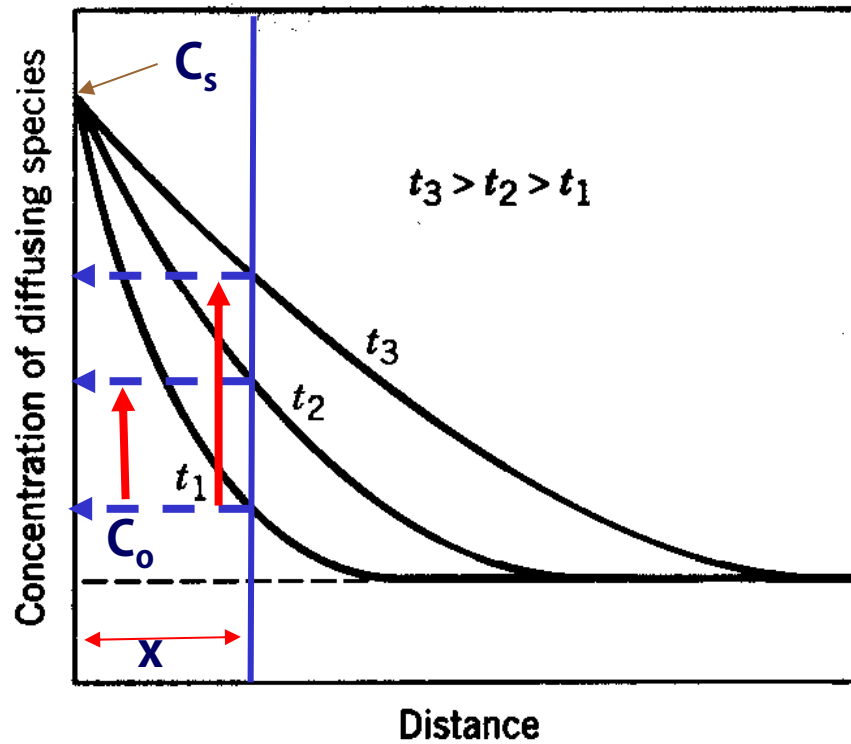
Non Steady State Diffusion

- steady-state diffusion not commonly encountered in engineering materials
- in most cases the concentration of solute atoms at any point in the material changes with time → **non-steady state diffusion**



Fick's Second Law

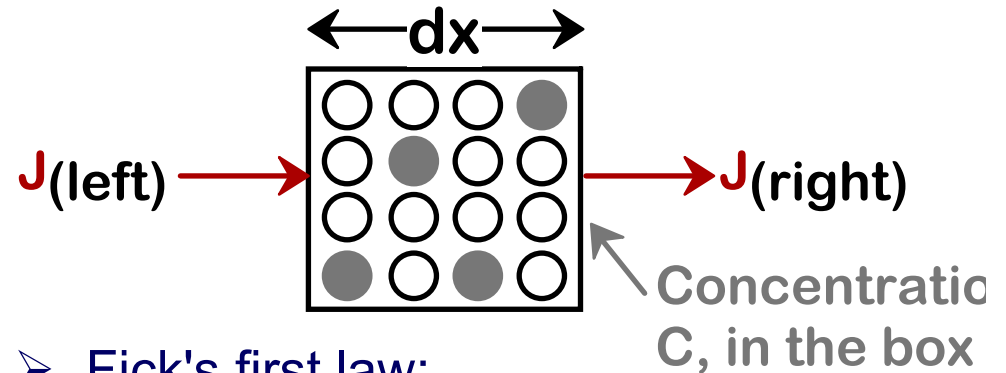
Fick's second law applies for non-steady state cases



$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial x} \left(D \frac{\partial C}{\partial x} \right)$$
$$\frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2}$$

Fick's Second Law

- Concentration profile, $C(x)$, changes w/ time



- To conserve matter:

$$\frac{J(\text{right}) - J(\text{left})}{dx} = - \frac{dC}{dt}$$

$$\frac{dJ}{dx} = - \frac{dC}{dt}$$

- Fick's first law:

$$J = -D \frac{dC}{dx} \quad \text{or}$$

$$\frac{dJ}{dx} = -D \frac{d^2C}{dx^2} \quad (\text{if } D \text{ does not vary with } x)$$

equate

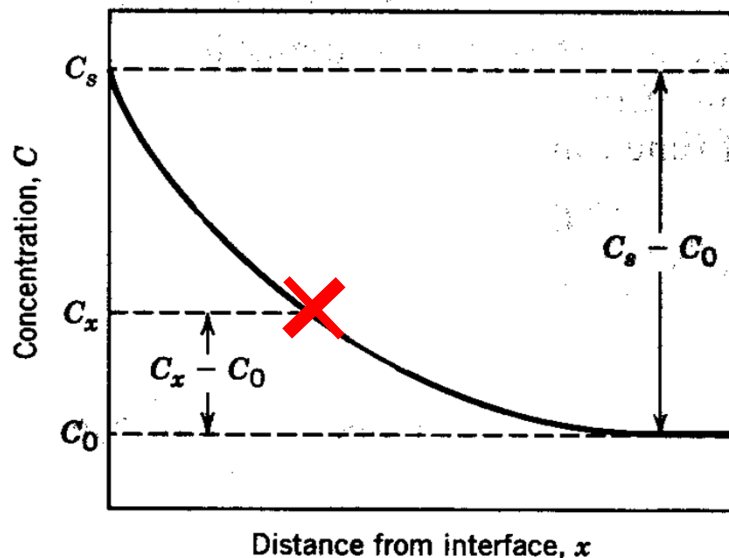
- Governing Eqn.:

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

- Fick's second law:

Fick's Second Law

- To solve Fick's second law, physically meaningful boundary conditions must be specified
- A practical and important solution is for a semi-infinite solid in which the surface concentration is held constant
- boundary conditions: For $t = 0, C = C_0$ at $0 \leq x \leq \infty$



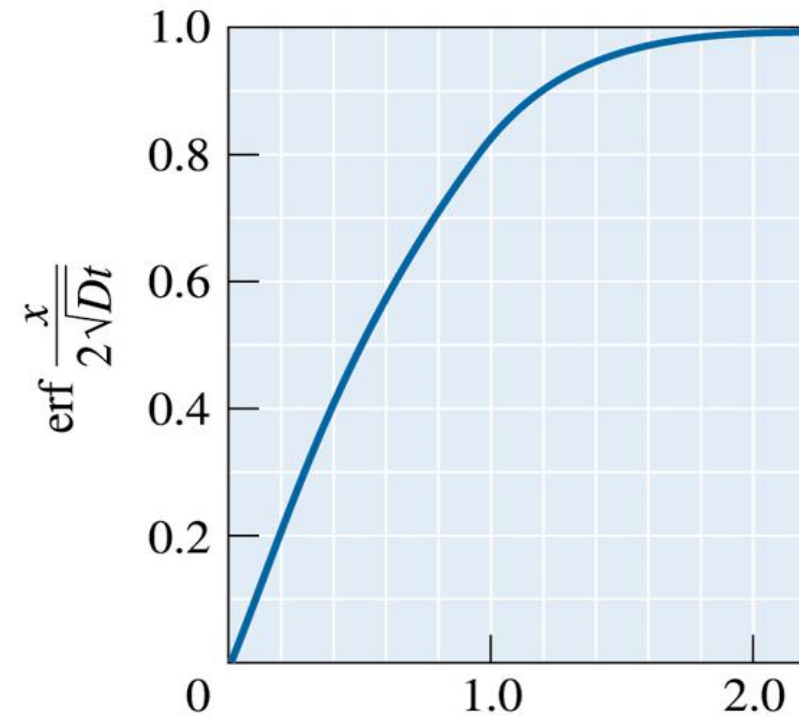
For $t > 0, C = C_s$ (the constant surface concentration) at $x = 0$

$$C = C_0 \text{ at } x = \infty$$

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

z	erf(z)	z	erf(z)
0.00	0.0000	0.70	0.6778
0.01	0.0113	0.75	0.7112
0.02	0.0226	0.80	0.7421
0.03	0.0338	0.85	0.7707
0.04	0.0451	0.90	0.7969
0.05	0.0564	0.95	0.8209
0.10	0.1125	1.00	0.8427
0.15	0.1680	1.10	0.8802
0.20	0.2227	1.20	0.9103
0.25	0.2763	1.30	0.9340
0.30	0.3286	1.40	0.9523
0.35	0.3794	1.50	0.9661
0.40	0.4284	1.60	0.9763
0.45	0.4755	1.70	0.9838
0.50	0.5205	1.80	0.9891
0.55	0.5633	1.90	0.9928
0.60	0.6039	2.00	0.9953
0.65	0.6420		

Error Function



effective penetration distance: $C(x_{eff}, t) = \frac{C_o + C_s}{2} \operatorname{erf}\left(\frac{x}{2\sqrt{Dt}}\right)$

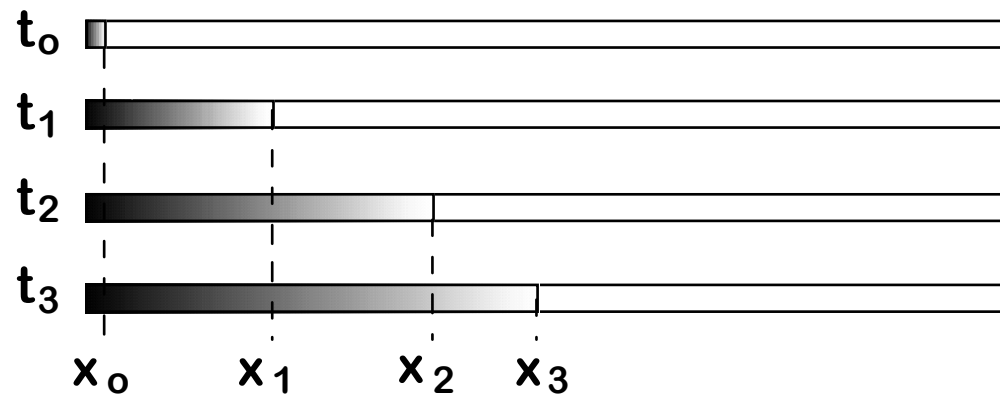
$$0.5 = \operatorname{erf}\left(\frac{x_{eff}}{2\sqrt{Dt}}\right) \quad \operatorname{erf}(0.5) \approx 0.5$$

$x_{eff} \approx \sqrt{Dt}$

in general $x_{eff} = \gamma\sqrt{Dt}$

Diffusion Demo: Analysis

- The experiment: we recorded combinations of t and x that kept C constant



$$\frac{C(x_i, t_i) - C_0}{C_s - C_0} = 1 - \operatorname{erf}\left(\frac{x_i}{2\sqrt{Dt_i}}\right) = (\text{constant here})$$

- Diffusion depth given by:

$$x_i \propto \sqrt{Dt_i}$$

Non-steady State Diffusion

- Copper diffuses into a bar of aluminum.

Surface conc.,
 C_S of Cu atoms

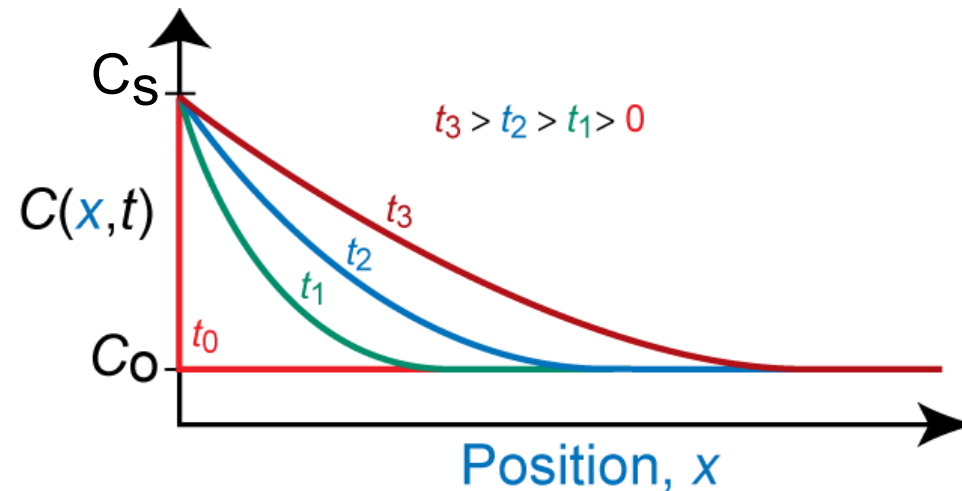
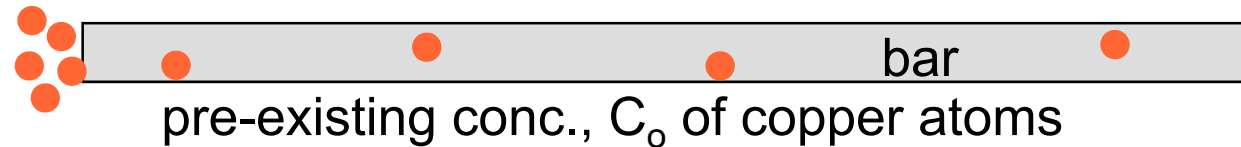


Fig. 7.5,
Callister &
Rethwisch 9e.

B.C. at $t = 0$, $C = C_0$ for $0 \leq x \leq \infty$

at $t > 0$, $C = C_S$ for $x = 0$ (constant surface conc.)

$C = C_0$ for $x = \infty$

Solution:

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

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

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

$$= \frac{2}{\sqrt{\pi}} \int_0^z e^{-y^2} dy$$

$\operatorname{erf}(z)$ values are given in Table 7.1

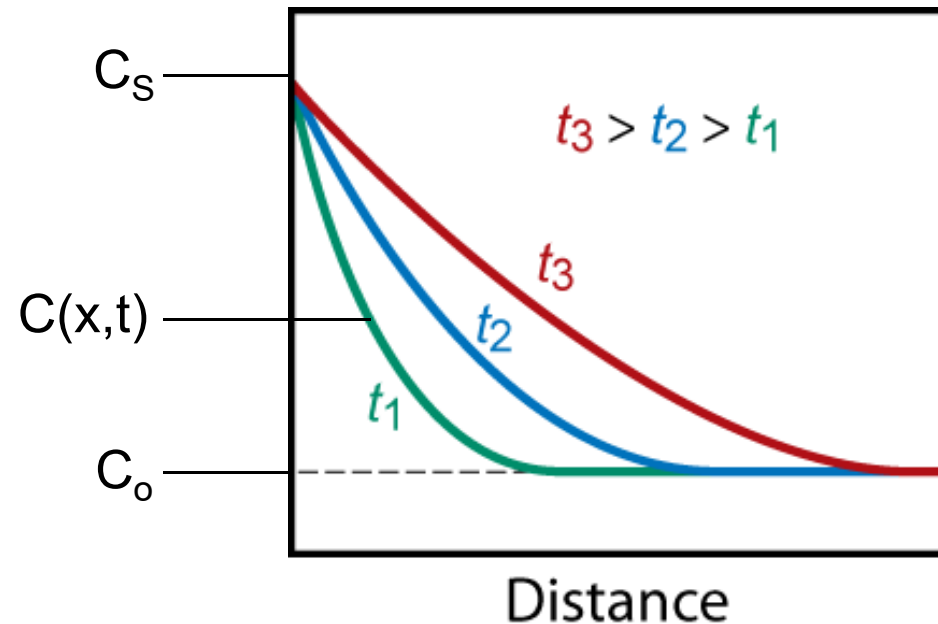


Fig. 7.5, Callister & Rethwisch 9e.

Example: Non-steady State Diffusion

- Sample Problem: An FCC iron-carbon alloy initially containing 0.20 wt% C is carburized at an elevated temperature and in an atmosphere that gives a surface carbon concentration constant at 1.0 wt%. If after 49.5 h the concentration of carbon is 0.35 wt% at a position 4.0 mm below the surface, determine the temperature at which the treatment was carried out.

- **Solution:** use Eqn. 7.5

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

Solution (cont.):

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

– $t = 49.5 \text{ h}$

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

– $C_x = 0.35 \text{ wt\%}$

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

– $C_o = 0.20 \text{ wt\%}$

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

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

Solution (cont.):

We must now determine from Table 7.1 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

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

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

Solution (cont.):

- To solve for the temperature at which D has the above value, we use a rearranged form of Equation (8.9a);

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

from Table 8.2, for diffusion of C in FCC Fe

$$D_o = 2.3 \times 10^{-5} \text{ m}^2/\text{s} \quad Q_d = 148,000 \text{ J/mol}$$

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

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

4. Factors Influencing Diffusion

- Temperature
- Diffusion Coefficient (D)
- Time
- Dependence on Bonding and Crystal Structure
- Types of Diffusion - volume diffusion, grain boundary diffusion, surface diffusion
- Dependence on Concentration of Diffusing Species and Composition of Matrix

4-I. Diffusion and Temperature

(a) Diffusion coefficient increases with increasing T

$$D = D_0 \exp\left(-\frac{Q_d}{RT}\right)$$

D = diffusion coefficient [m²/s]

D₀ = pre-exponential [m²/s]

Q_d = activation energy [J/mol or eV/atom]

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

T = absolute temperature [K]

Diffusion Exercise

Example: Determine D_{Cu} in Ni at 500°C.

$$Q_d = 256 \text{ kJ/mol}$$

$$D_0 = 2.7 \times 10^{-5} \text{ m}^2/\text{sec}$$

$$T = 500 + 273 = 773 \text{ K}$$

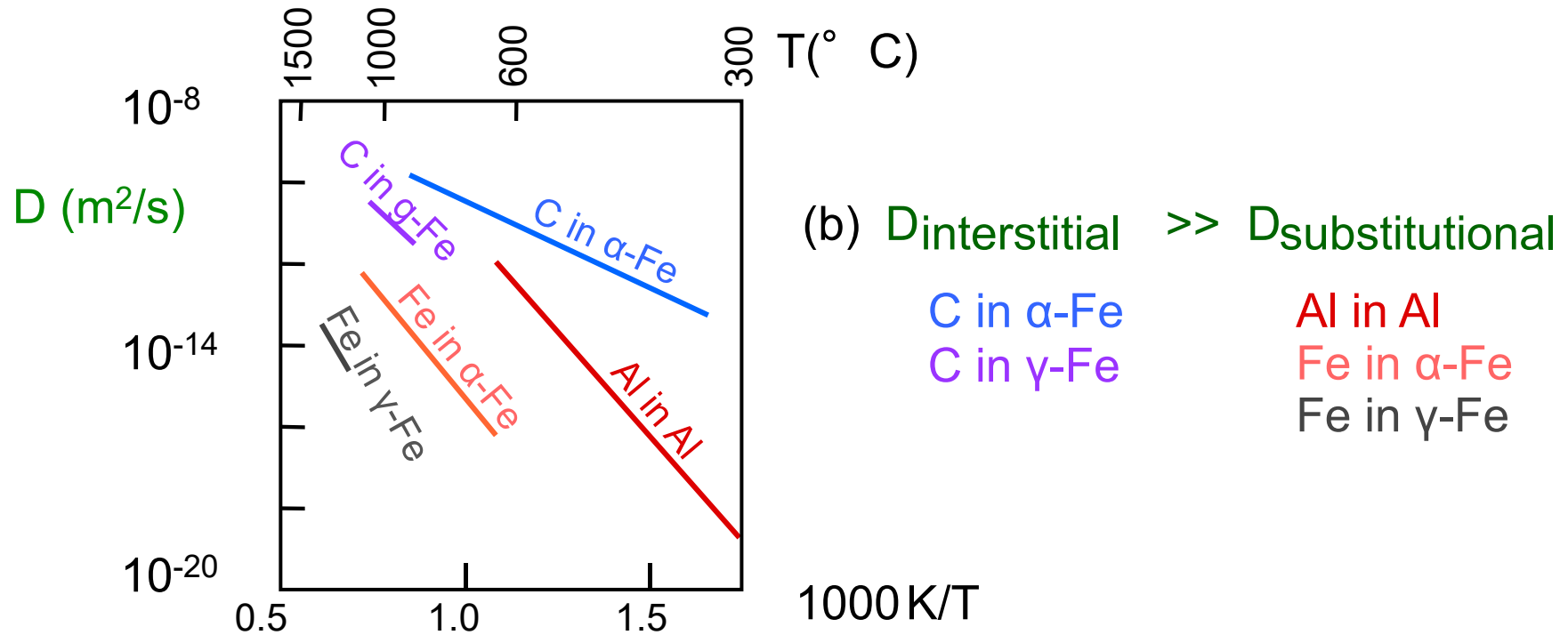
$$R = 8.31 \text{ J/mol-K}$$

$$D = 2.7 \times 10^{-5} \cdot \exp\left(-\frac{256000}{8.31 \times 773}\right)$$

$$D = 1.33 \times 10^{-22} \text{ m}^2/\text{sec}$$

4-I. Diffusion and Temperature

D has exponential dependence on T



Adapted from Fig. 7.7, Callister & Rethwisch 9e.
 (Data for Fig. 7.7 taken from E.A. Brandes and G.B. Brook (Ed.) Smithells Metals Reference Book, 7th ed., Butterworth-Heinemann, Oxford, 1992.)

Table 7.2

<i>Diffusing Species</i>	<i>Host Metal</i>	$D_0(m^2/s)$	$Q_d(J/mol)$
Interstitial Diffusion			
C ^b	Fe (α or BCC) ^a	1.1×10^{-6}	87,400
C ^c	Fe (γ or FCC) ^a	2.3×10^{-5}	148,000
N ^b	Fe (α or BCC) ^a	5.0×10^{-7}	77,000
N ^c	Fe (γ or FCC) ^a	9.1×10^{-5}	168,000
Self-Diffusion			
Fe ^c	Fe (α or BCC) ^a	2.8×10^{-4}	251,000
Fe ^c	Fe (γ or FCC) ^a	5.0×10^{-5}	284,000
Cu ^d	Cu (FCC)	2.5×10^{-5}	200,000
Al ^c	Al (FCC)	2.3×10^{-4}	144,000
Mg ^c	Mg (HCP)	1.5×10^{-4}	136,000
Zn ^c	Zn (HCP)	1.5×10^{-5}	94,000
Mo ^d	Mo (BCC)	1.8×10^{-4}	461,000
Ni ^d	Ni (FCC)	1.9×10^{-4}	285,000
Interdiffusion (Vacancy)			
Zn ^c	Cu (FCC)	2.4×10^{-5}	189,000
Cu ^c	Zn (HCP)	2.1×10^{-4}	124,000
Cu ^c	Al (FCC)	6.5×10^{-5}	136,000
Mg ^c	Al (FCC)	1.2×10^{-4}	130,000
Cu ^c	Ni (FCC)	2.7×10^{-5}	256,000
Ni ^d	Cu (FCC)	1.9×10^{-4}	230,000

^aThere are two sets of diffusion coefficients for iron because iron experiences a phase transformation at 912°C; at temperatures less than 912°C, BCC α -iron exists; at temperatures higher than 912°C, FCC γ -iron is the stable phase.

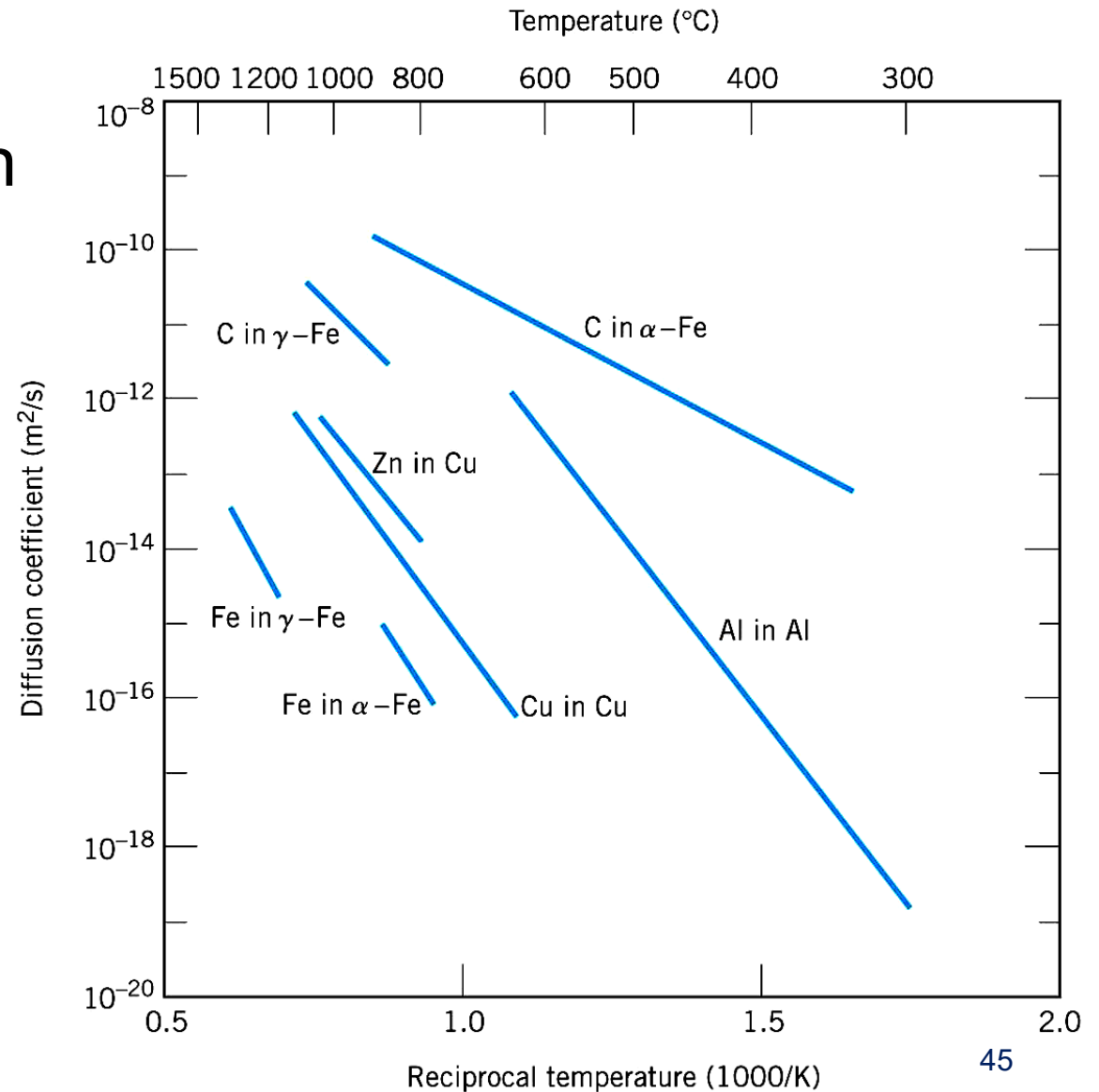
^bY. Adda and J. Philibert, *Diffusion Dans Les Solides*, Universitaires de France, Paris, 1966.

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

^dJ. Askill, *Tracer Diffusion Data for Metals, Alloys, and Simple Oxides*, IFI/Plenum, New York, 1970.

Factors Influencing Diffusion temperature

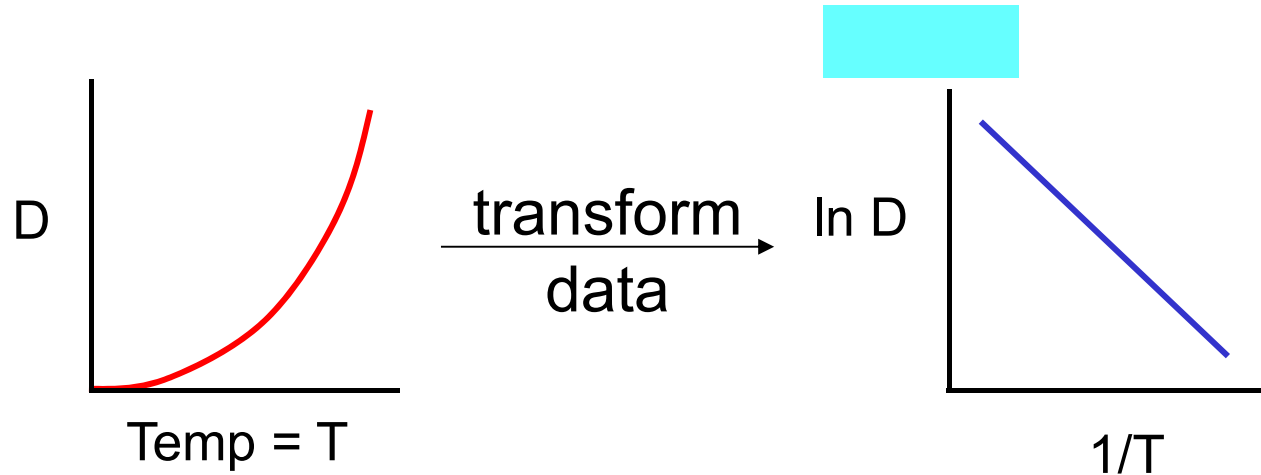
- **Arrhenius plot** of relationship between diffusion coefficient and reciprocal of temperature for different elements



Example: At 300° C the diffusion coefficient and activation energy for Cu in Si are

$$D(300^\circ \text{ C}) = 7.8 \times 10^{-11} \text{ m}^2/\text{s}, \quad Q_d = 41.5 \text{ kJ/mol}$$

(c) What is the diffusion coefficient at 350° C?



$$\ln D_2 = \ln D_0 - \frac{Q_d}{R} \left(\frac{1}{T_2} \right) \quad \text{and} \quad \ln D_1 = \ln D_0 - \frac{Q_d}{R} \left(\frac{1}{T_1} \right)$$

$$\therefore \ln D_2 - \ln D_1 = \ln \frac{D_2}{D_1} = -\frac{Q_d}{R} \left(\frac{1}{T_2} - \frac{1}{T_1} \right)$$

Example (cont.)

$$D_2 = D_1 \exp \left[-\frac{Q_d}{R} \left(\frac{1}{T_2} - \frac{1}{T_1} \right) \right]$$

$$T_1 = 273 + 300 = 573 \text{ K}$$

$$T_2 = 273 + 350 = 623 \text{ K}$$

$$D_2 = (7.8 \times 10^{-11} \text{ m}^2/\text{s}) \exp \left[\frac{-41,500 \text{ J/mol}}{8.314 \text{ J/mol-K}} \left(\frac{1}{623 \text{ K}} - \frac{1}{573 \text{ K}} \right) \right]$$

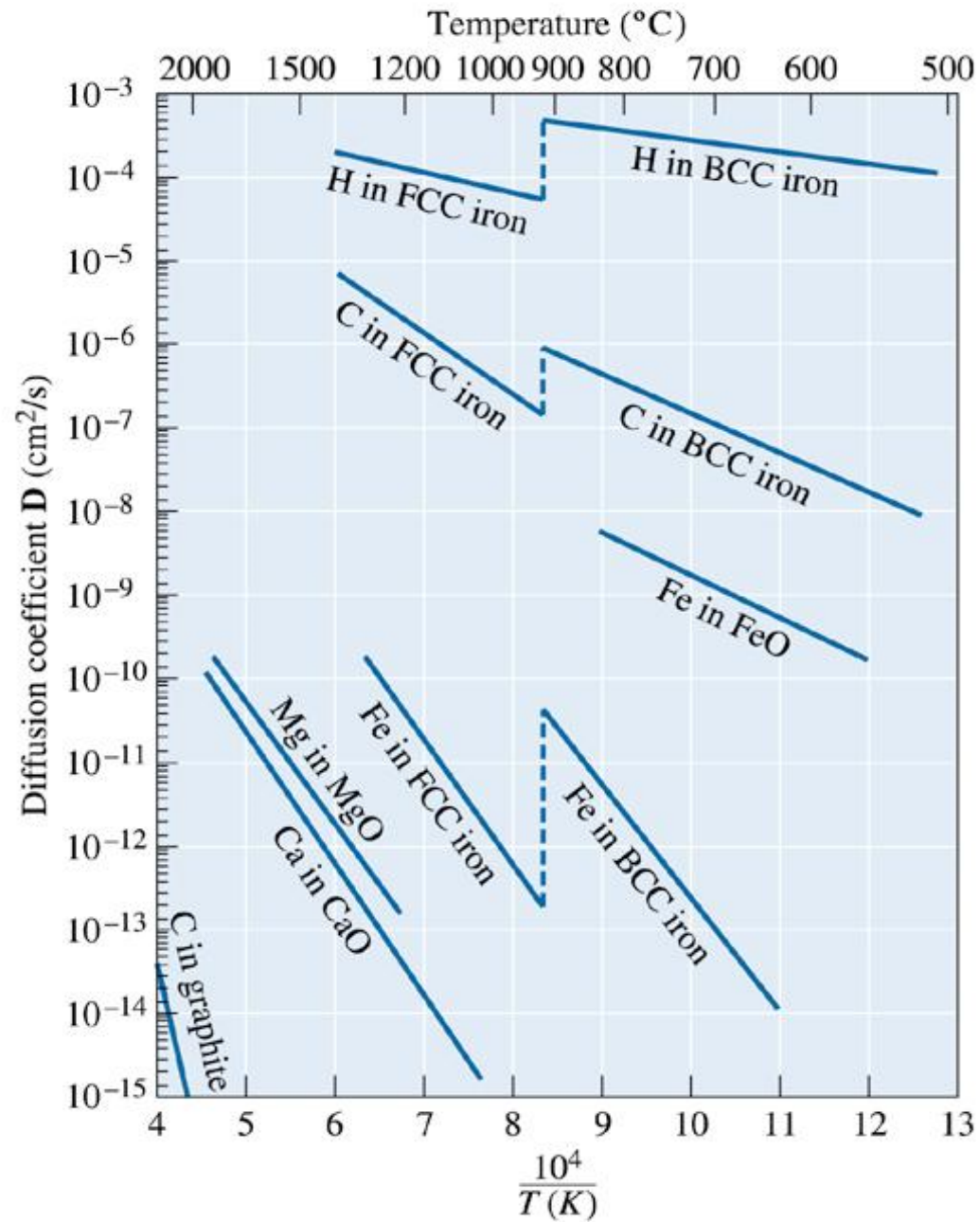
$$D_2 = 15.7 \times 10^{-11} \text{ m}^2/\text{s}$$

4-II. Factors Influencing Diffusion crystal structure

- The crystal structure of the metal affects the diffusion rate:
 - Diffusivities of different elements in BCC-Fe are higher than in FCC-Fe at the same temperature (e.g. 910°C)
 - Reasons for faster diffusion in BCC compared with FCC iron
 - BCC iron lattice is slightly more open; it has lower packing factor than FCC
 - BCC lattice has a coordination number of 8 compared with 12 in FCC
→ fewer bonds must be broken when elements diffuse in BCC iron

Diffusivities of various elements in BCC and FCC iron at 910 °C

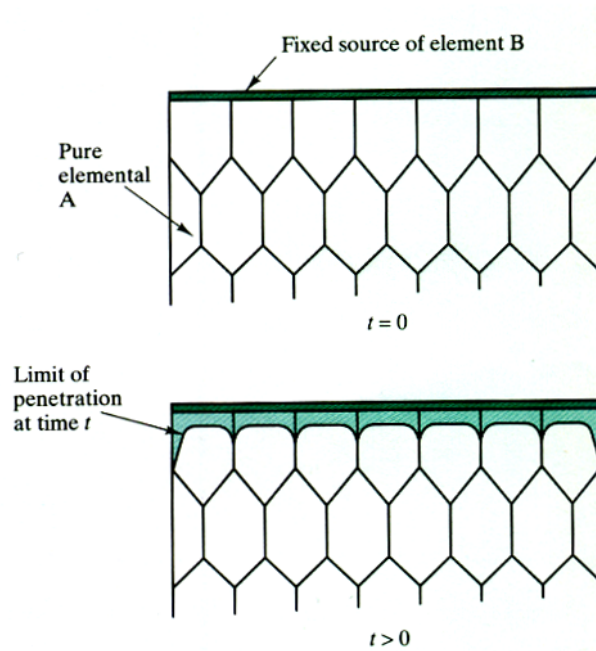
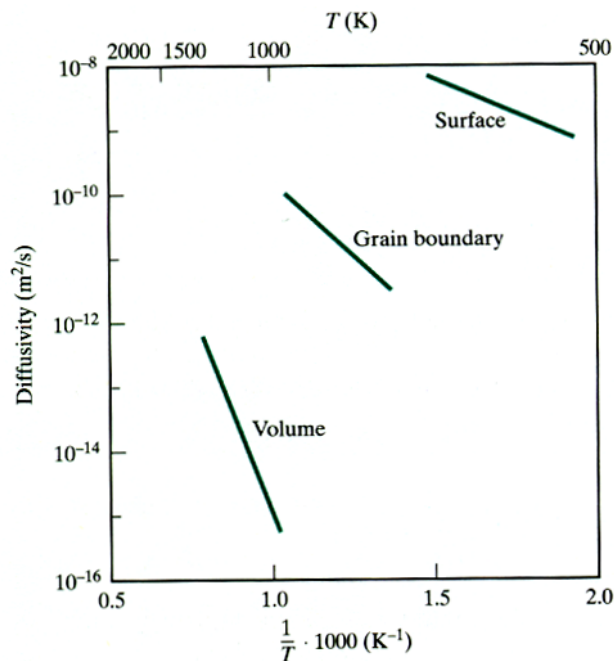
Solute	D in BCC Fe, cm ² /s	D in FCC Fe, cm ² /s	Solute	D in BCC Fe, cm ² /s	D in FCC Fe, cm ² /s
Al	1.3×10^{-10}	...	Mn . . .	7.0×10^{-11}	4.8×10^{-13}
Be . . .	1.3×10^{-9}	2.8×10^{-12}	N	7.5×10^{-5}	...
C	3.9×10^{-5}	1.1×10^{-7}	Ni	5.9×10^{-11}	3.2×10^{-13}
Co . . .	2.9×10^{-11}	4.8×10^{-14}	S	2.1×10^{-8}	2.7×10^{-10}
Cr	6.0×10^{-11}	1.4×10^{-12}	Sb . . .	5.5×10^{-10}	...
Cu . . .	4×10^{-11}	...	Si	8.1×10^{-11}	5.7×10^{-12}
Fe . . .	4.5×10^{-11}	1.4×10^{-13}	Ti	4.0×10^{-11}	1.2×10^{-12}
Mo . . .	2.5×10^{-10}	1.3×10^{-12}	W	1.9×10^{-12}	5.0×10^{-13}



← Increase in Temperature

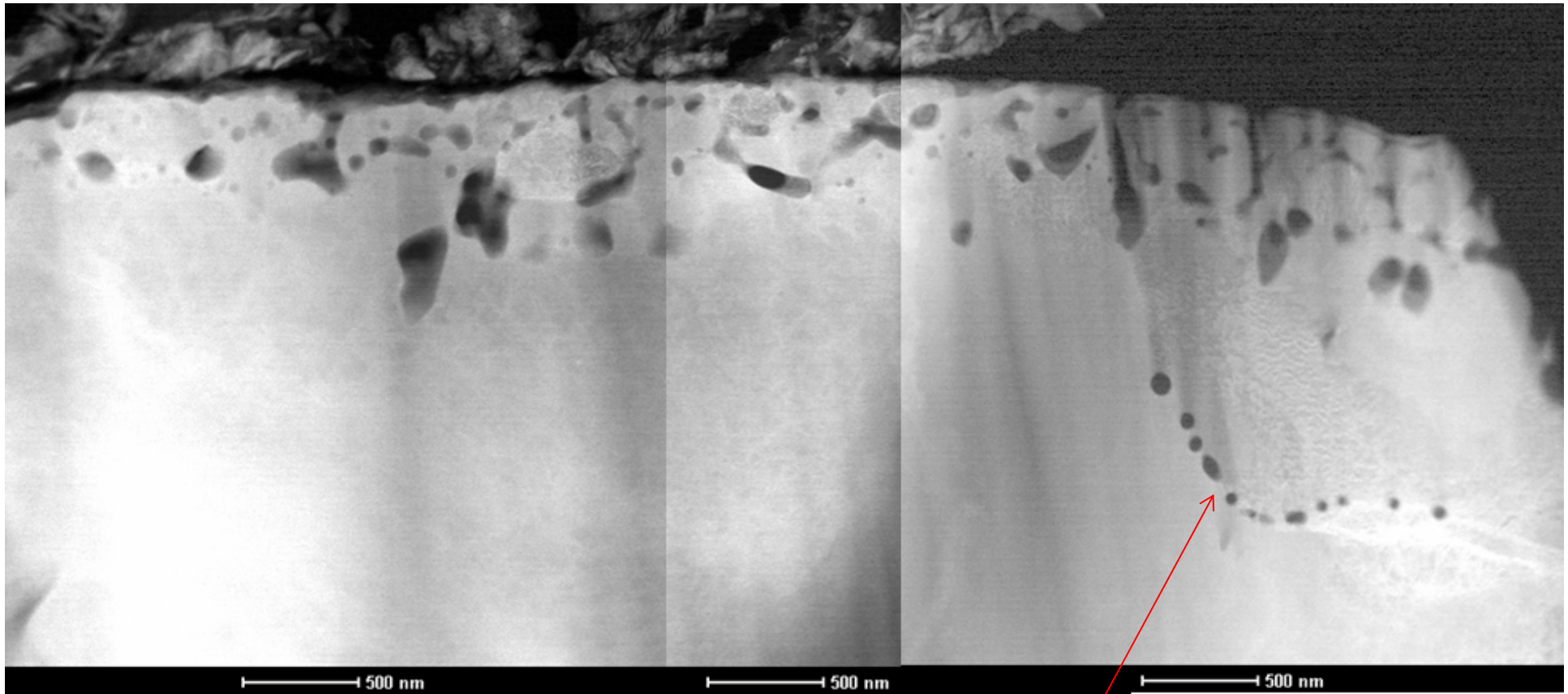
III. Factors Influencing Diffusion_grain boundary

- Diffusion is faster along grain boundaries than through grains:
 - More open structure at grain boundaries than the interior grain
 - Much lower activation energy for diffusion in grain boundaries compared to transgranular diffusion



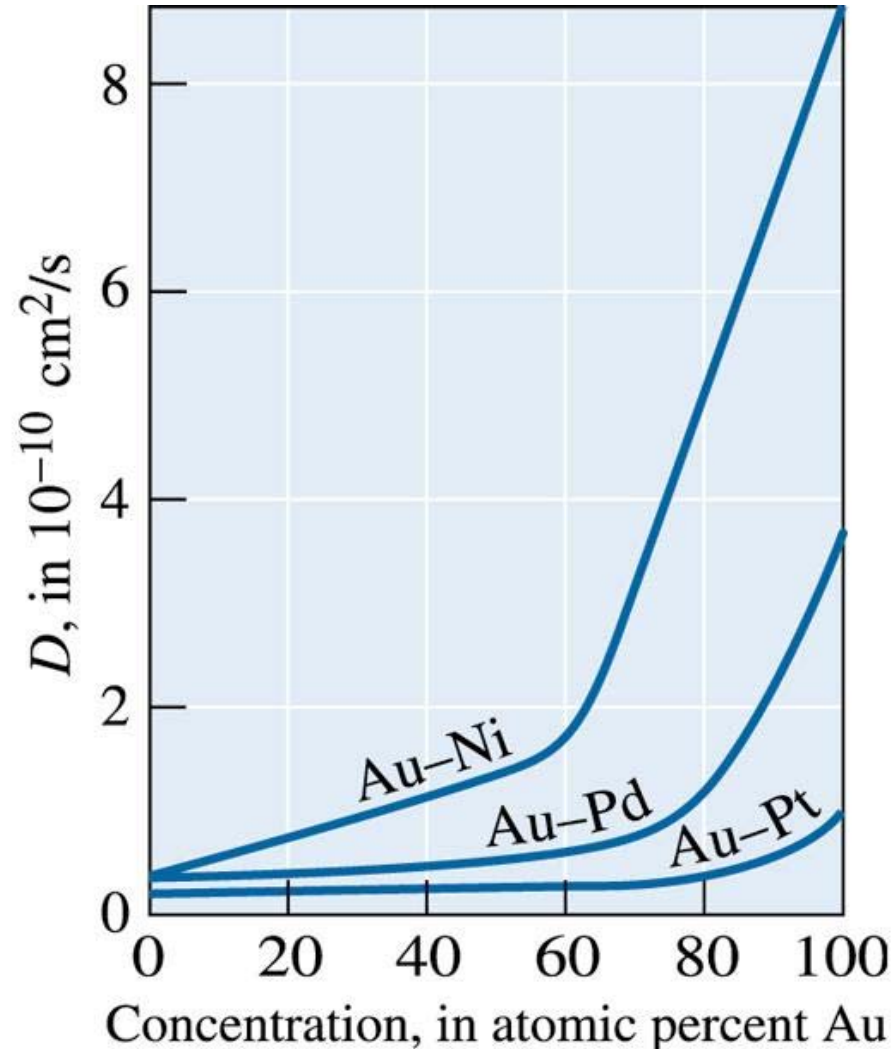
$$Q_{\text{volume}} > Q_{\text{gb}} > Q_{\text{surface}}$$
$$D_{\text{volume}} < D_{\text{gb}} < D_{\text{surface}}$$

Oxidation – Grainboundary diffusion



Grain boundary

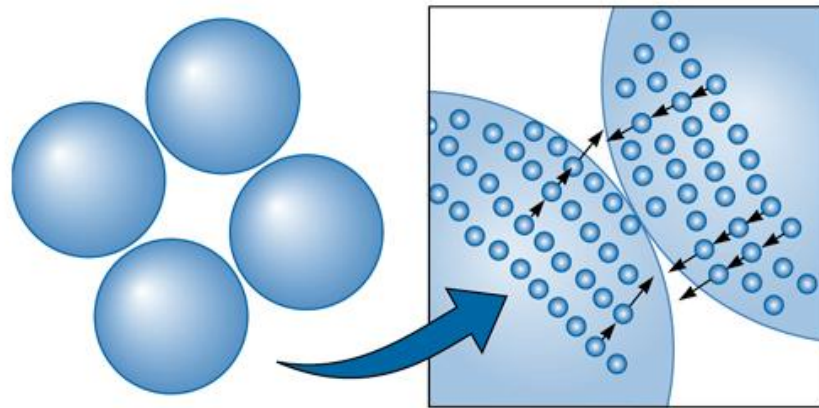
IV. Factors Influencing Diffusion : concentration of diffusing species



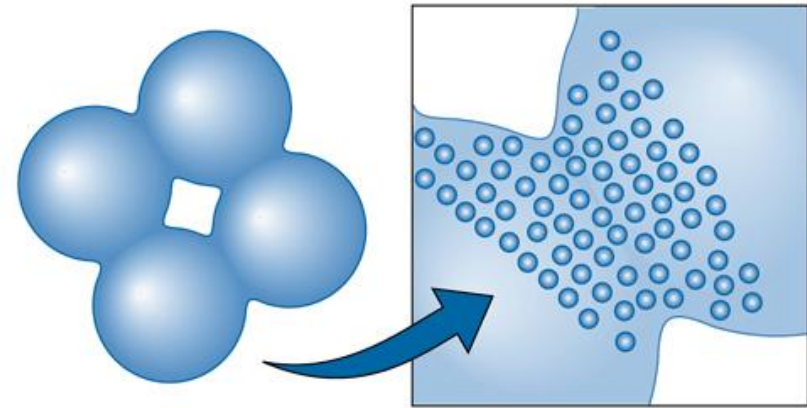
The dependence of diffusion coefficient of Au on concentration of Au

5. Diffusion and Materials Processing

- **Sintering** - A high-temperature treatment used to join small particles
- **Powder metallurgy** - A method for producing monolithic metallic parts
- **Grain growth** - Movement of grain boundaries by diffusion in order to reduce the amount of grain boundary area
- **Diffusion bonding** - A joining technique in which two surfaces are pressed together at high pressures and temperatures



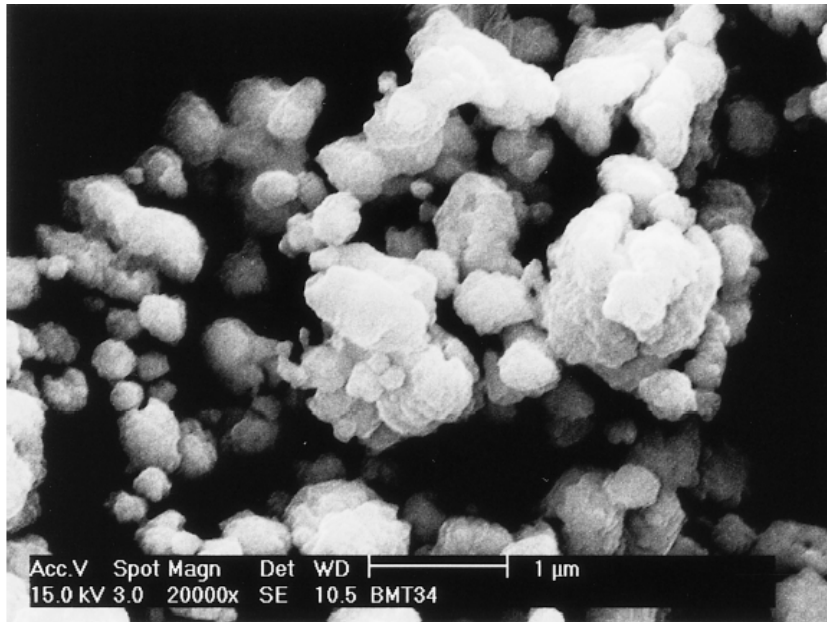
Compacted product



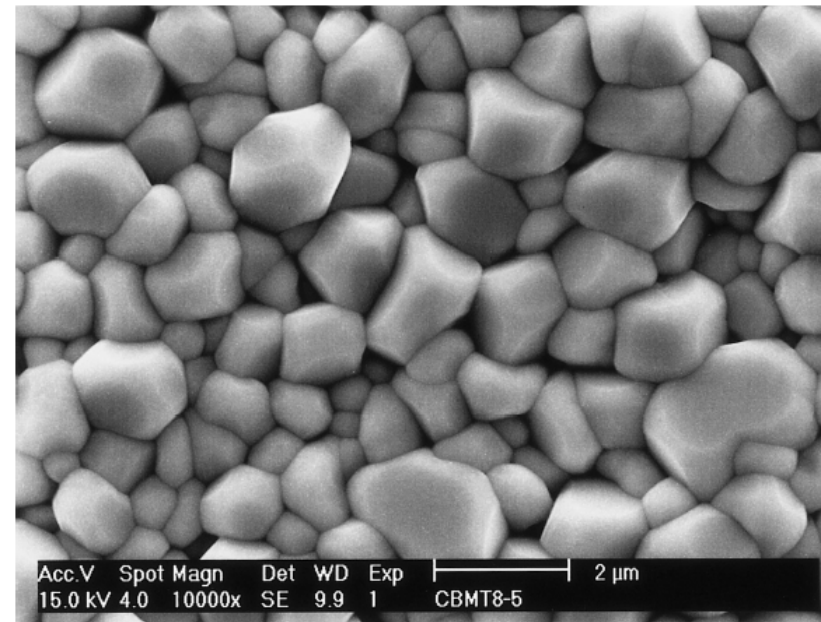
Partly sintered product

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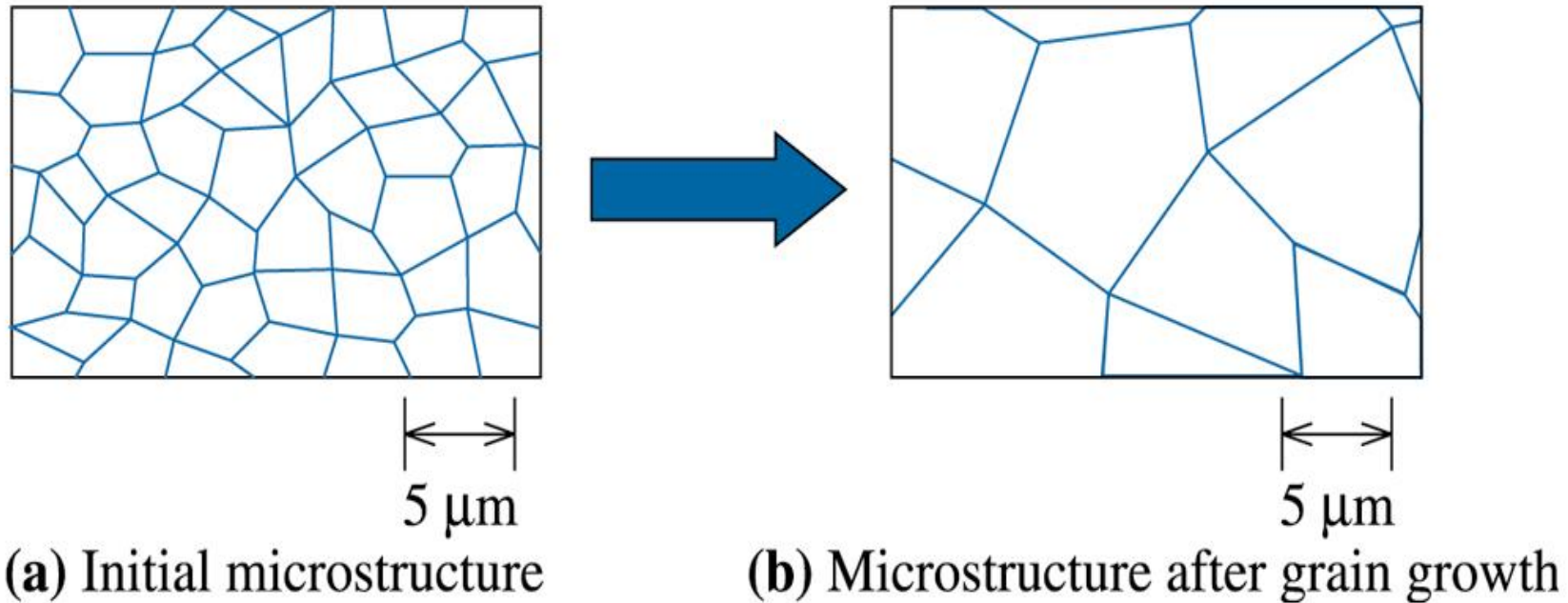
(a, b) Diffusion processes during **sintering and powder metallurgy**. Atoms diffuse to points of contact, creating bridges and reducing the pore size



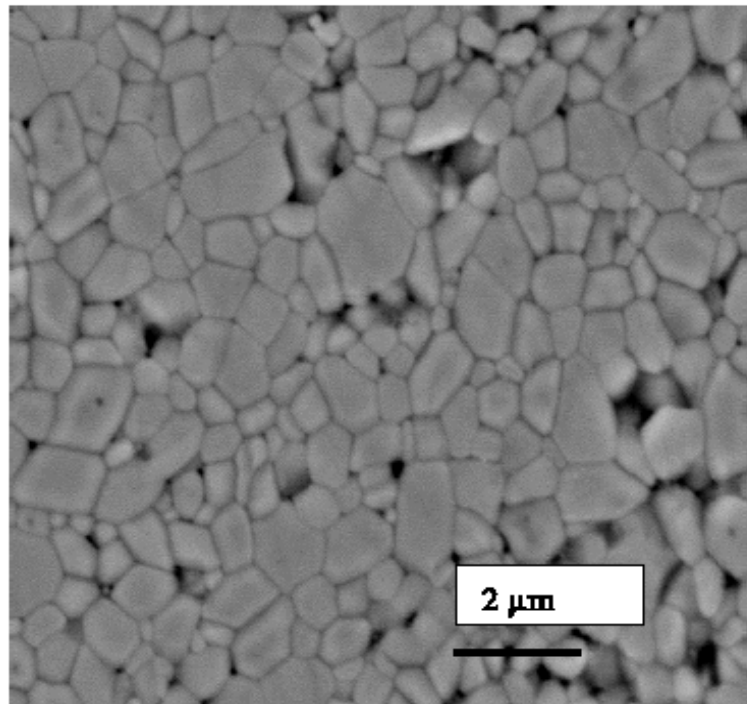
Particles of barium magnesium tantalate (BMT) ($\text{Ba}(\text{Mg}_{1/3}\text{Ta}_{2/3})\text{O}_3$) powder are shown. This ceramic material is useful in making electronic components known as dielectric resonators that are used for wireless communications.



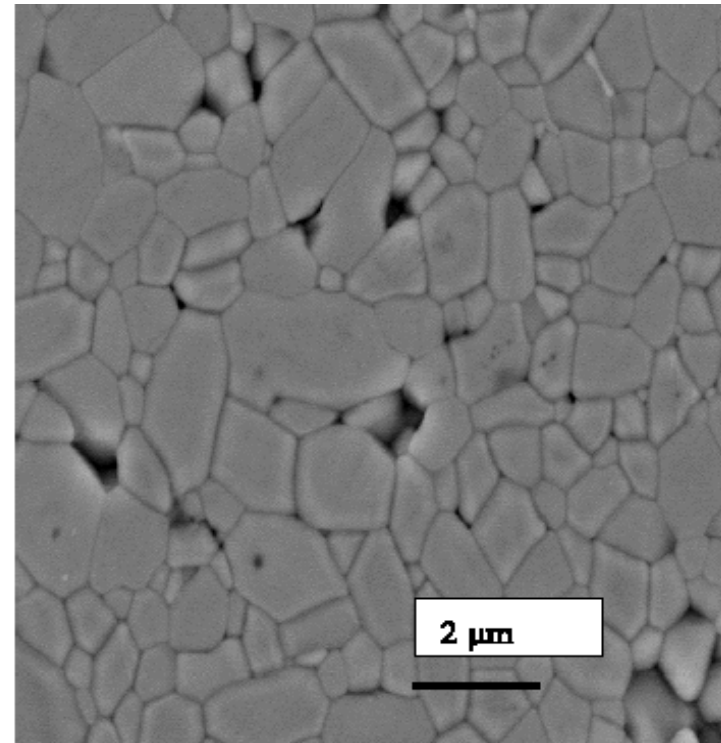
The microstructure of BMT ceramics obtained by compaction and **sintering** of BMT powders.



Grain growth occurs as atoms diffuse across the grain boundary from one grain to another

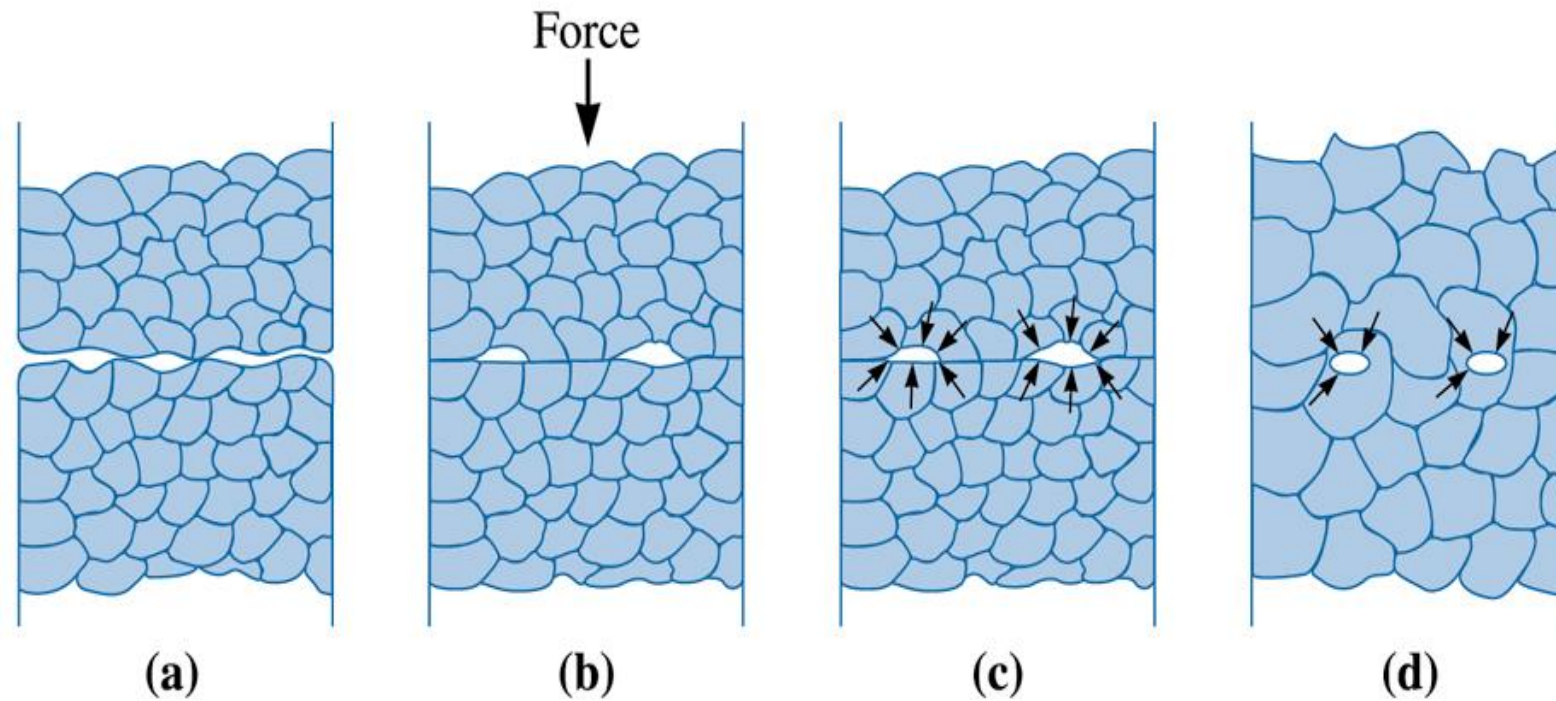


(a)



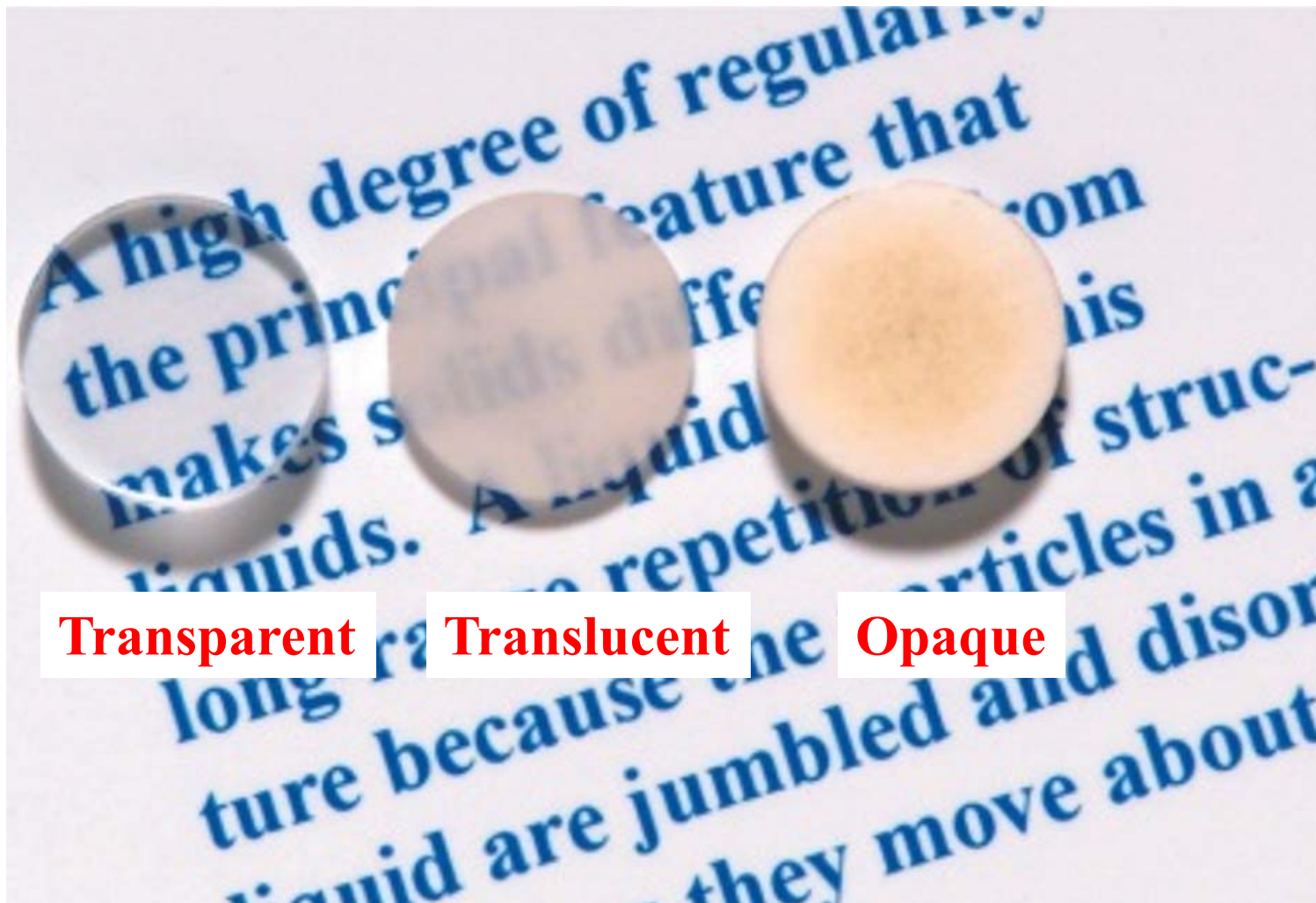
(b)

Grain growth in alumina ceramics can be seen from the SEM micrographs of alumina ceramics. (a) The left micrograph shows the microstructure of an alumina ceramic sintered at 1350°C for 150 hours. (b) The right micrograph shows a sample sintered at 1350°C for 300 hours.



The steps in **diffusion bonding**: (a) Initially the contact area is small; (b) application of pressure deforms the surface, increasing the bonded area; (c) grain boundary diffusion permits voids to shrink; and (d) final elimination of the voids requires volume diffusion

Void Effect on the optical properties



SUMMARY: Structure & Diffusion

1. Fick's First law: $J = -D \frac{dC}{dx}$ 2. Fick's Second law: $\frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2}$

3. Estimation of Diffusion Depth: 4. Diffusion coefficient:

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

$$D = D_0 \exp\left(\frac{Q_d}{RT}\right)$$

Diffusion FASTER for...	Diffusion SLOWER for...
open crystal structures	close-packed structures
lower melting T materials	higher melting T materials
materials w/secondary bonding	materials w/covalent bonding
smaller diffusing atoms	larger diffusing atoms
cations	anions
lower density materials	higher density materials