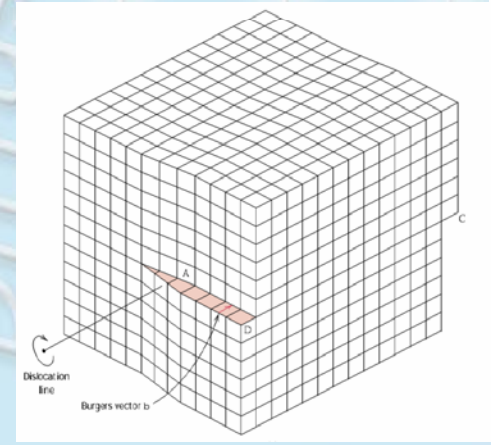
Linear defects are also called *dislocations*

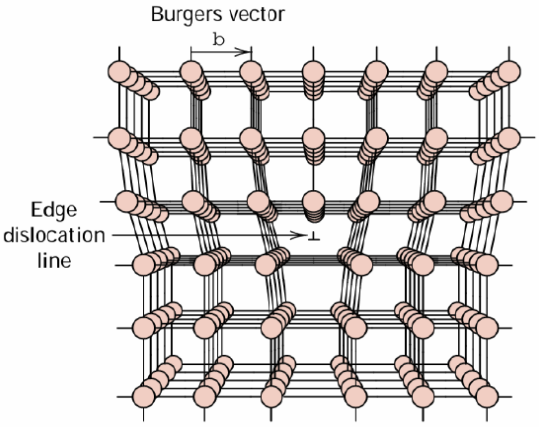
We will distinguish two types of dislocations:

- Edge dislocations

Notice the relative positions of the dislocation lines with respect to the Burgers vectors

- Screw dislocations





The nature of a dislocation (edge, screw, or mixed) is defined by the relative orientations of dislocation line and Burgers vector.
For metallic materials, the Burgers vector for a dislocation will point in a close-packed crystallographic direction and will be of magnitude equal to the interatomic spacing.

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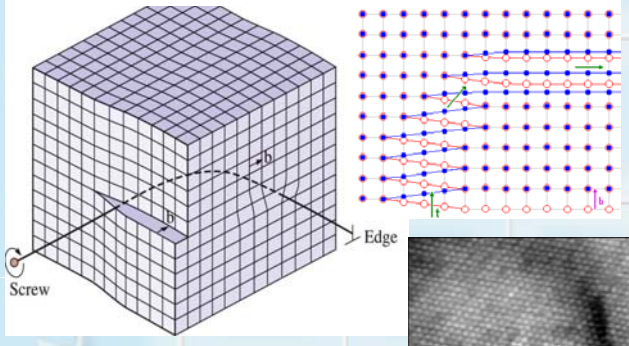
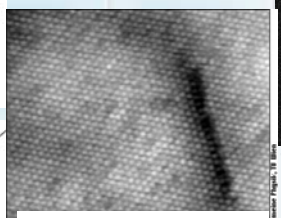
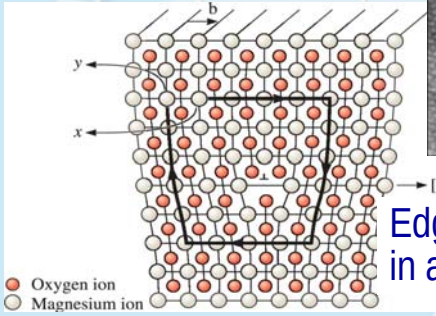
More Dislocations

More common situation: mixed dislocations





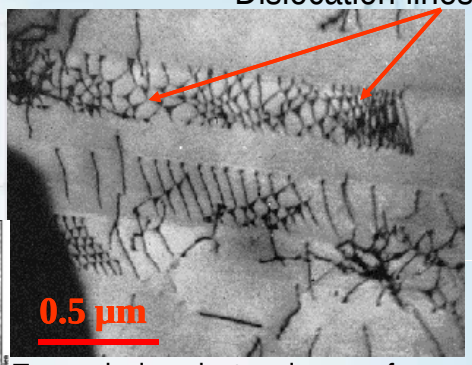
STM image of screw dislocation



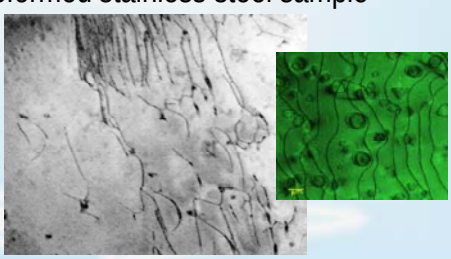
Edge Dislocation in an MgO crystal

Physical Evidence of Dislocations

Dislocation lines

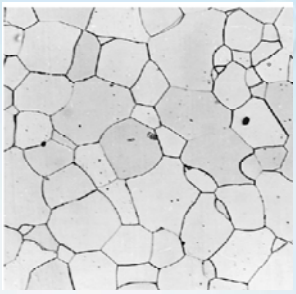


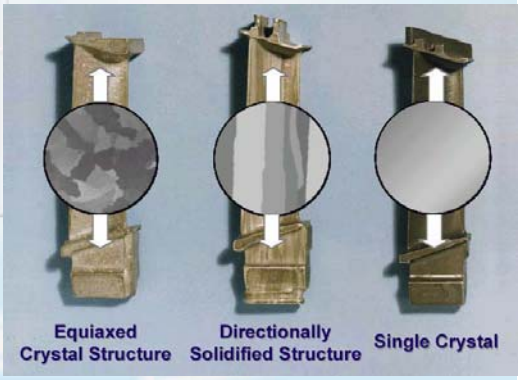
Transmission electron image of a deformed stainless steel sample



Surface Defects or Grain Boundaries

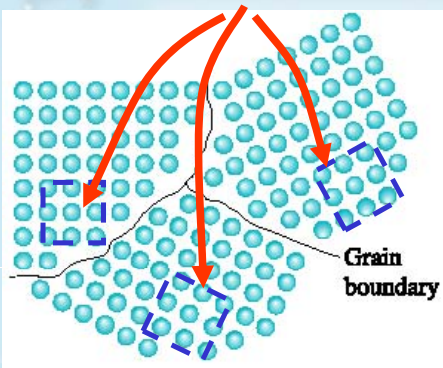
- Granular structure of crystalline solids
  - Each grain differentiates itself from the neighbor only in its crystalline orientation
  - Each grain meets its neighbors along *grain boundaries*.
- Study of all defects can be done through microscopy

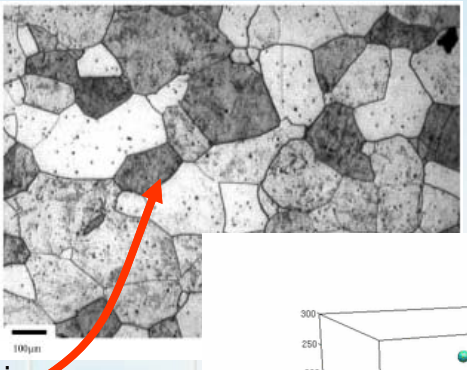




Grain Boundaries

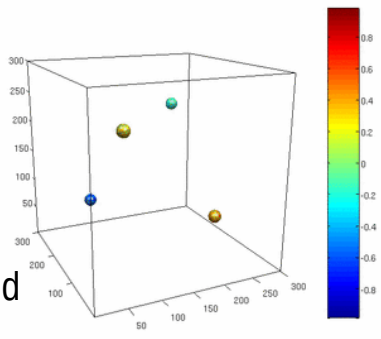
Observe what happens when at three different points in space crystals form and grow (propagate) in every direction.



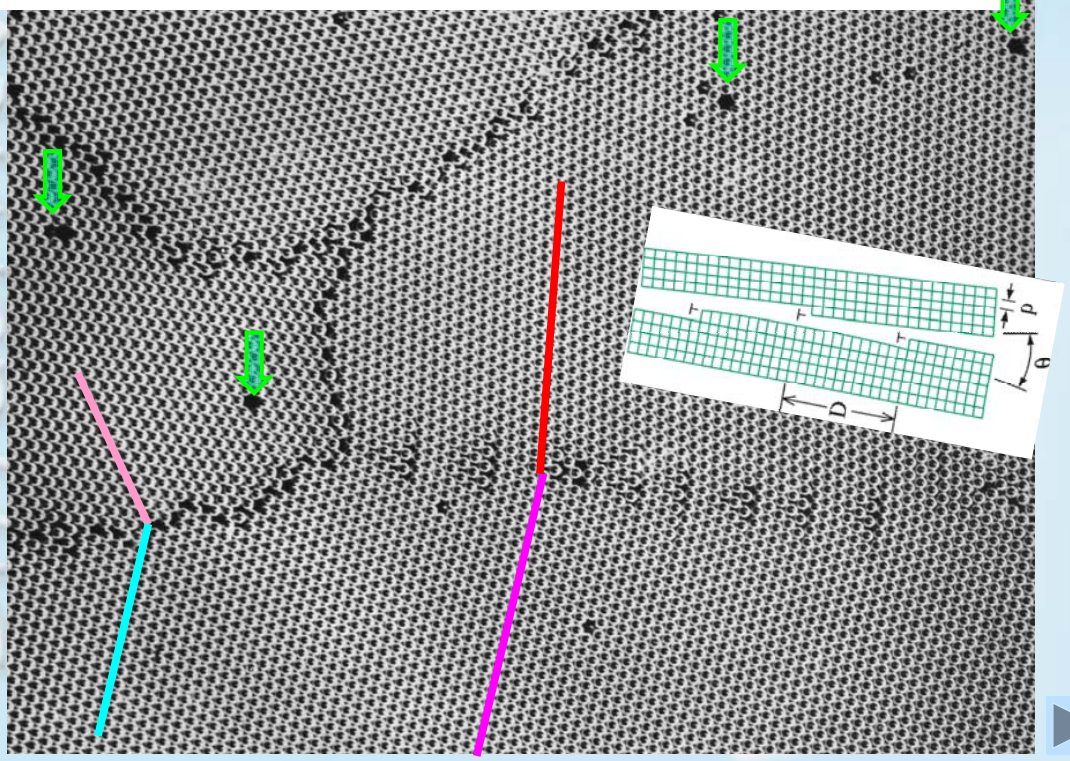


Grain boundaries are zone of grain impingement into each other.

In this 3D simulation, several crystals nucleate and start growing with different spatial orientations.

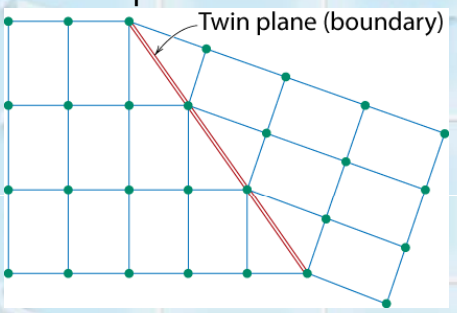


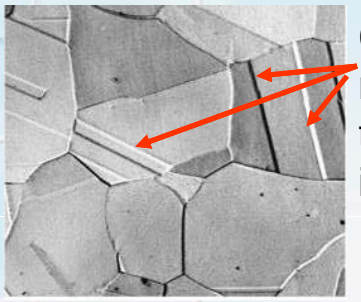
The Bubble Raft Experiment



Other Planar Defects in Solids

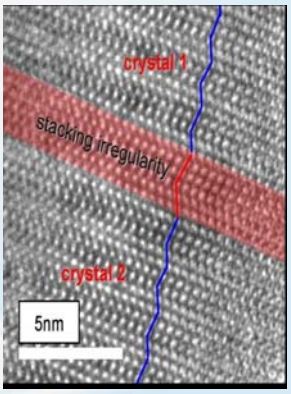
- Twinning
  - Essentially a reflection of atom positions across the twin plane.





Optical micrograph of twinnings in pure iron

- Stacking faults
  - For FCC metals an error in ABCABC packing sequence
  - Ex: ABCABABC, Aluminum is a good example of a material with low stacking fault energy



Chapter 5

Atom and Ion Movements in Materials

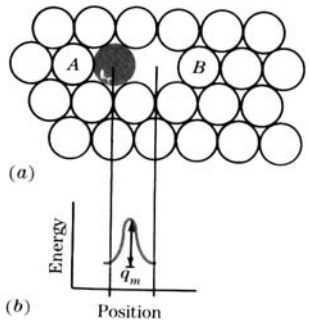
Diffusion

Diffusion in Solids

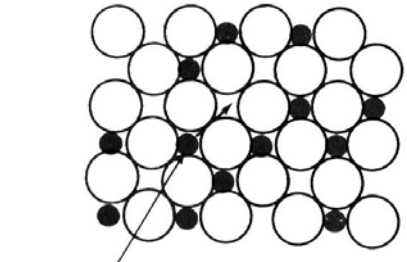
- Similarities with diffusion in liquids and gases
- Diffusion mechanisms:
  - Substitutional diffusion: requires vacancies!
    - In pure elements → self-diffusion (random walk)
  - Interstitial diffusion: "channels" for diffusion can be smaller

Let's differentiate between diffusion mechanisms.

Substitutional Diffusion:

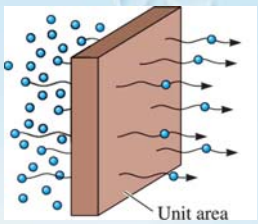


Interstitial Diffusion:



Diffusion in Solids (cont.)

- The mobility is a property of the material
- The driving force is a gradient of certain physical magnitude



In the presence of a concentration gradient:

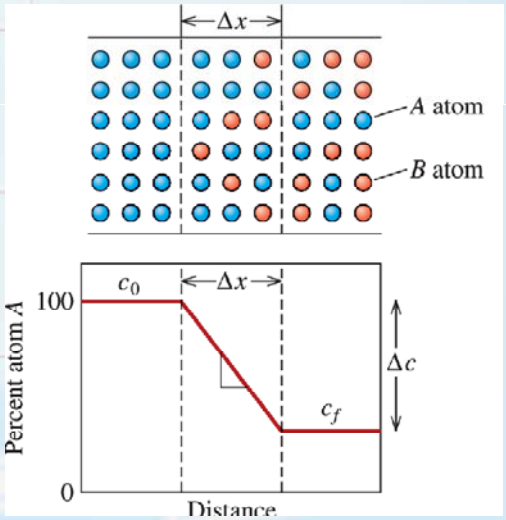
Flux of atoms

$$J = -D \cdot \frac{\partial C}{\partial x}$$

Diffusivity of atoms

Concentration gradient

Fick's First Law of Diffusion



Variables Affecting Diffusion

- Type of diffusion mechanism: substitutional or interstitial
- Temperature
- Crystal structure of the solvent
- Crystal imperfections present
- Concentration of diffusing species

Non-steady State Diffusion

When the concentration gradient is not fixed in time we need another equation:

Fick's Second Law of Diffusion:

$$\frac{\partial C_x}{\partial t} = \frac{\partial}{\partial}\left(D \cdot \frac{\partial C_x}{\partial x}\right)$$

If D is constant (rough simplification):

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

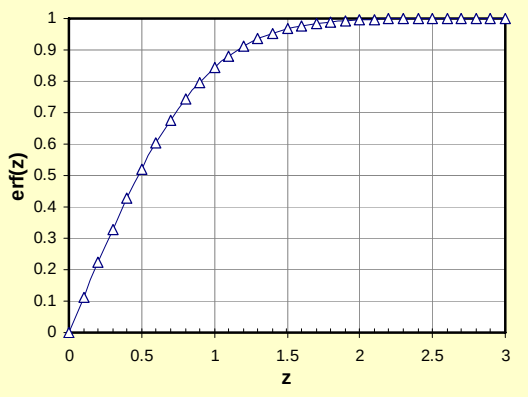
Non-steady State Diffusion (cont.)

For this differential equation there's a solution after imposing some initial conditions:

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

$$\frac{C_s - C_x}{C_s - C_0} = \text{erf}\left(\frac{x}{2\cdot\sqrt{D\cdot t}}\right)$$

erf: error function



And the terms in the equation mean:

$$\frac{C_s - C_x}{C_s - C_0} = \text{erf}\left(\frac{x}{2\cdot\sqrt{D\cdot t}}\right)$$

C_s: Concentration at the surface (assumed to be constant during the entire process

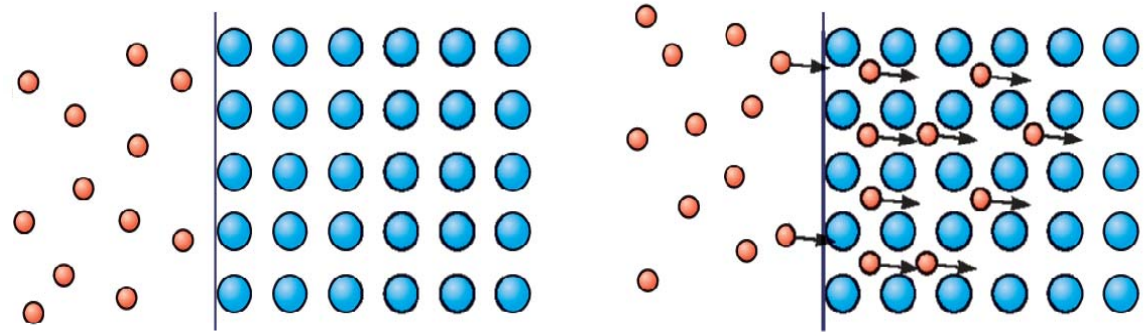
C_0: Initial uniform concentration

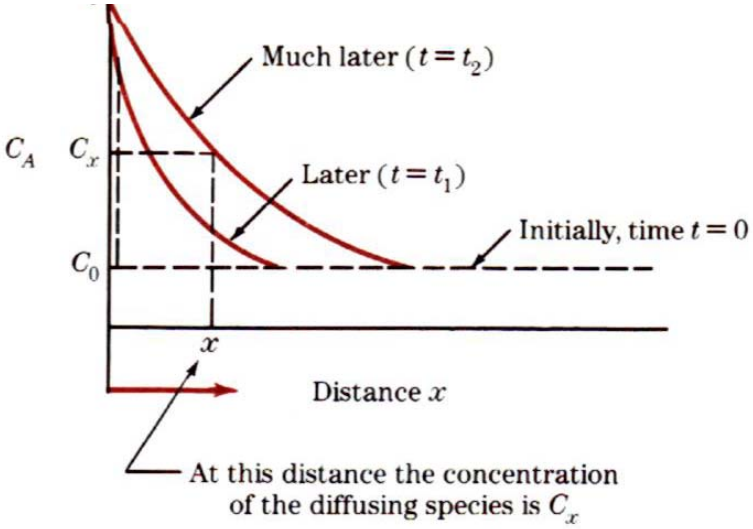
C_x: Concentration at a distance x

x: distance from the surface

t: diffusion time

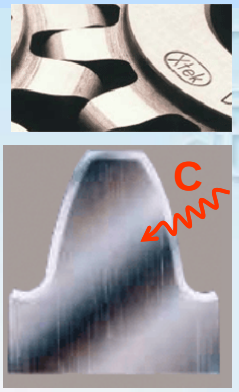
D: diffusivity of solute element





Example

Determine the carburizing time necessary to achieve a carbon concentration of 0.45 wt.% at a position 2mm into an iron-carbon alloy that initially contains 0.20 wt.% C. The surface concentration is to be maintained at 1.30wt.%C and the treatment is to be conducted at 1000ºC. For carbon diffusing into γFe: $D_0 = 2.3 \cdot 10^{-5}$ m^2/s and Q = 148 kJ/mol or look at the plot of diffusivities.



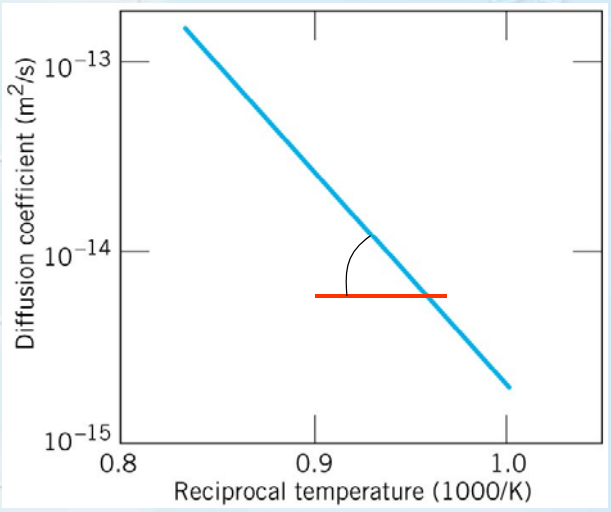
z	erf z	z	erf z	z	erf z	z	erf z
0	0	0.40	0.4284	0.85	0.7707	1.6	0.9763
0.025	0.0282	0.45	0.4755	0.90	0.7970	1.7	0.9838
0.05	0.0564	0.5	0.5205	0.95	0.8209	1.8	0.9891
0.10	0.1125	0.55	0.5633	1.0	0.8427	1.9	0.9928
0.15	0.1680	0.6	0.6039	1.1	0.8802	2.0	0.9953
0.20	0.2227	0.65	0.6420	1.2	0.9103	2.2	0.9981
0.25	0.2763	0.70	0.6778	1.3	0.9340	2.4	0.9993
0.30	0.3286	0.75	0.7112	1.4	0.9523	2.6	0.9998
0.35	0.3794	0.80	0.7421	1.5	0.9661	2.8	0.9999

Temperature has a huge influence in Diffusion

Diffusivities (or diffusion coefficients) follow an Arrhenius equation:

$$D = D_0 \cdot e^{-\frac{Q}{RT}}$$

$$\ln D = \ln D_0 - \frac{Q}{R} \cdot \left(\frac{1}{T}\right)$$



Units of diffusivity: m^2/s

What is the value of R? Units?

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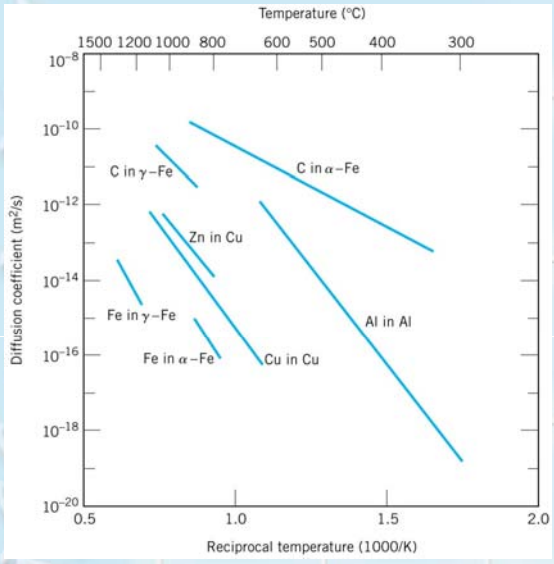
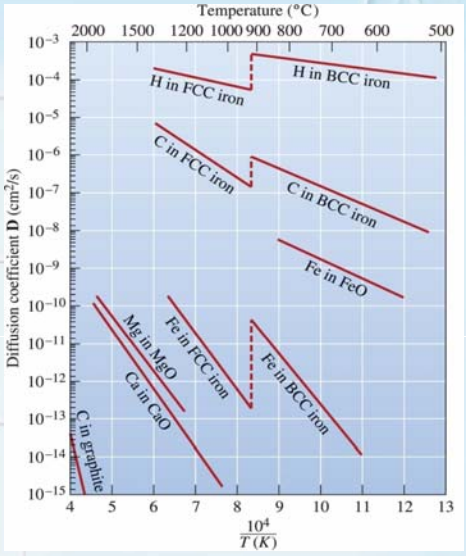
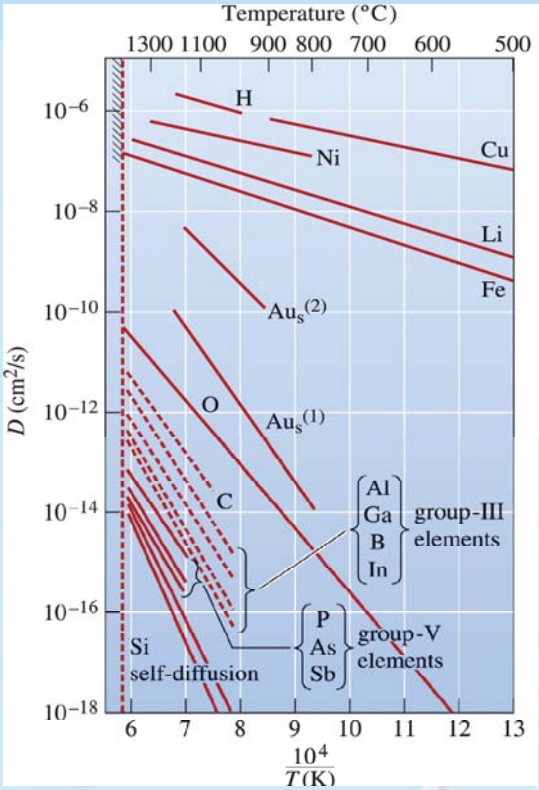
Arrhenius Plot of Diffusivities in Metals and other Materials





Draw some conclusions on the effect of the following factors on diffusivity:

Crystal structure; grain boundaries; solute atom size; point defects



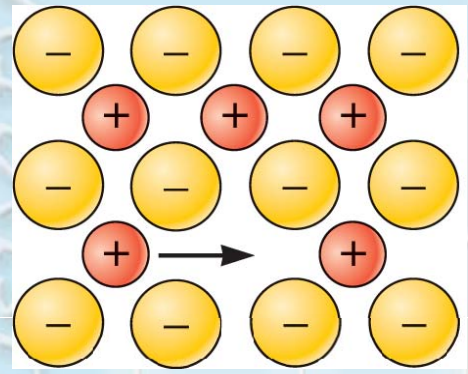
Diffusivities of various elements (dopants) in silicon

Note the effect of:

- Nature of the chemical bond
- Dopant atom size

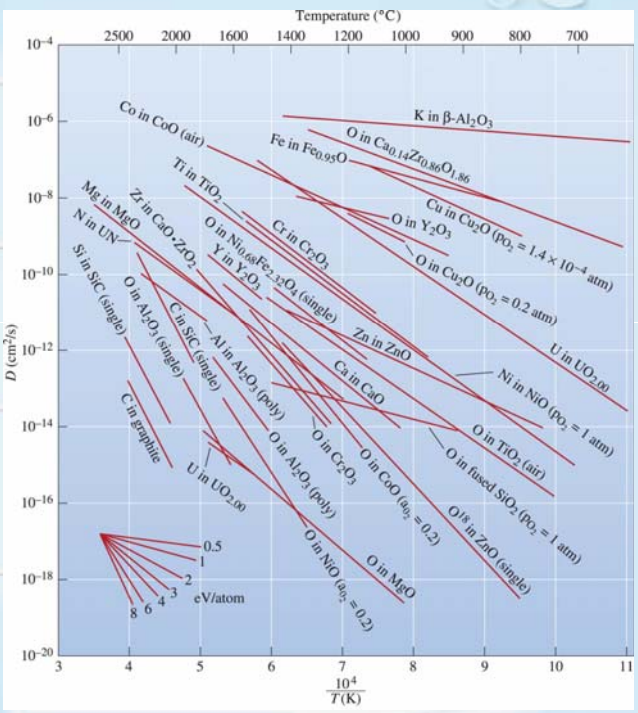
Why do you think group IV elements diffuse less in silicon than group III?

Diffusion in Ionic and More Covalent Solids

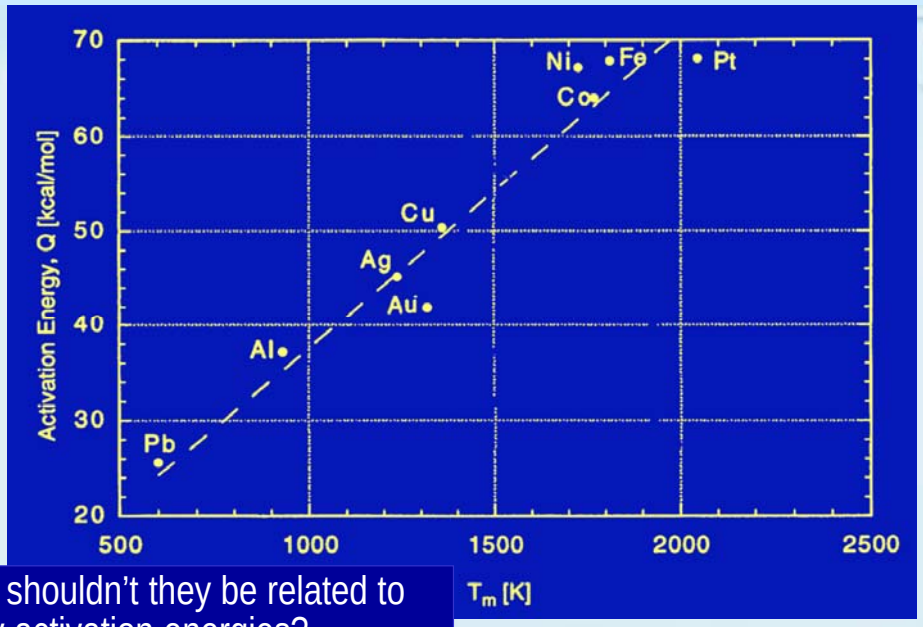


Effect of Schottky and Frenkel defects.

Ionic conductivity and diffusion in ionic solids are intimately related



This graph shows how activation energies for self diffusivities are related to melting points



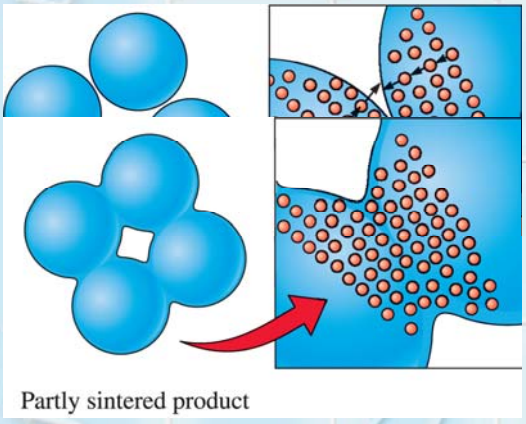
By the way, shouldn't they be related to the vacancy activation energies?

Summary: Structure and Diffusion

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

Two examples of diffusion processing in manufacturing

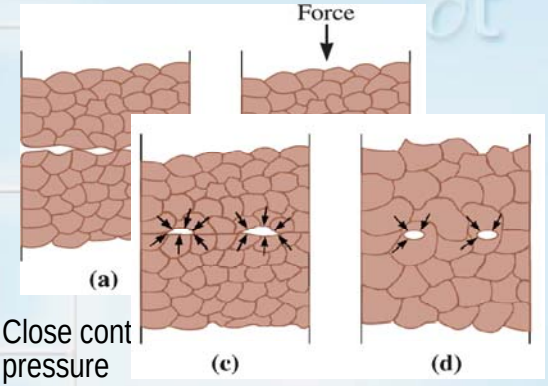
Compaction and sintering of powder (metal or ceramic)



How can you accelerate the process?

Investigate the application of powder metallurgy in rearview mirror mounts

Diffusion bonding (not welding)



Close cont
pressure

Grain boundary diffusion first.

Volume diffusion next (grain growth) eliminates pores

How can you enhance the process?