Department of Civil Engineering
IIT Madras

Movement of Atoms in Solids

Modern Construction Materials – Lecture 4
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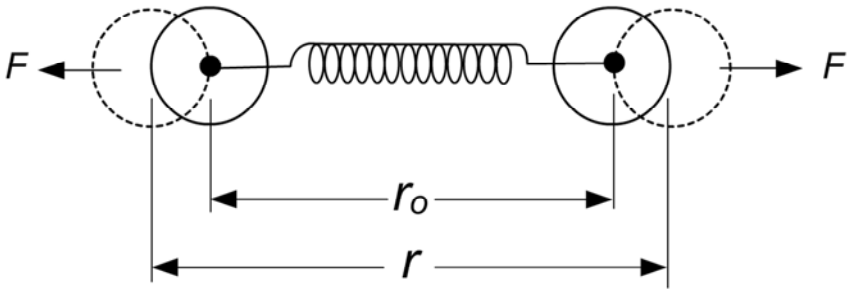
Movement of Atoms in the Lattice

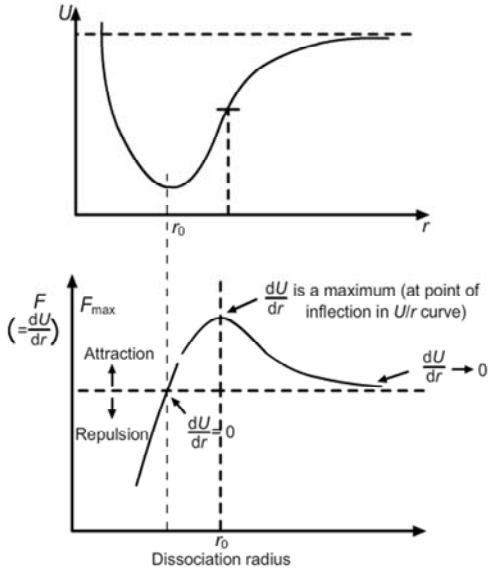


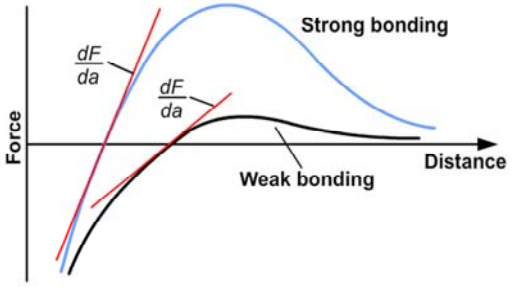
When there are small changes in interatomic spacing due to the stretching of interatomic bonds, the deformation is elastic (i.e., non-permanent).

Ashby & Jones, Callister

Movement of Atoms in the Lattice

Interatomic forces and distances





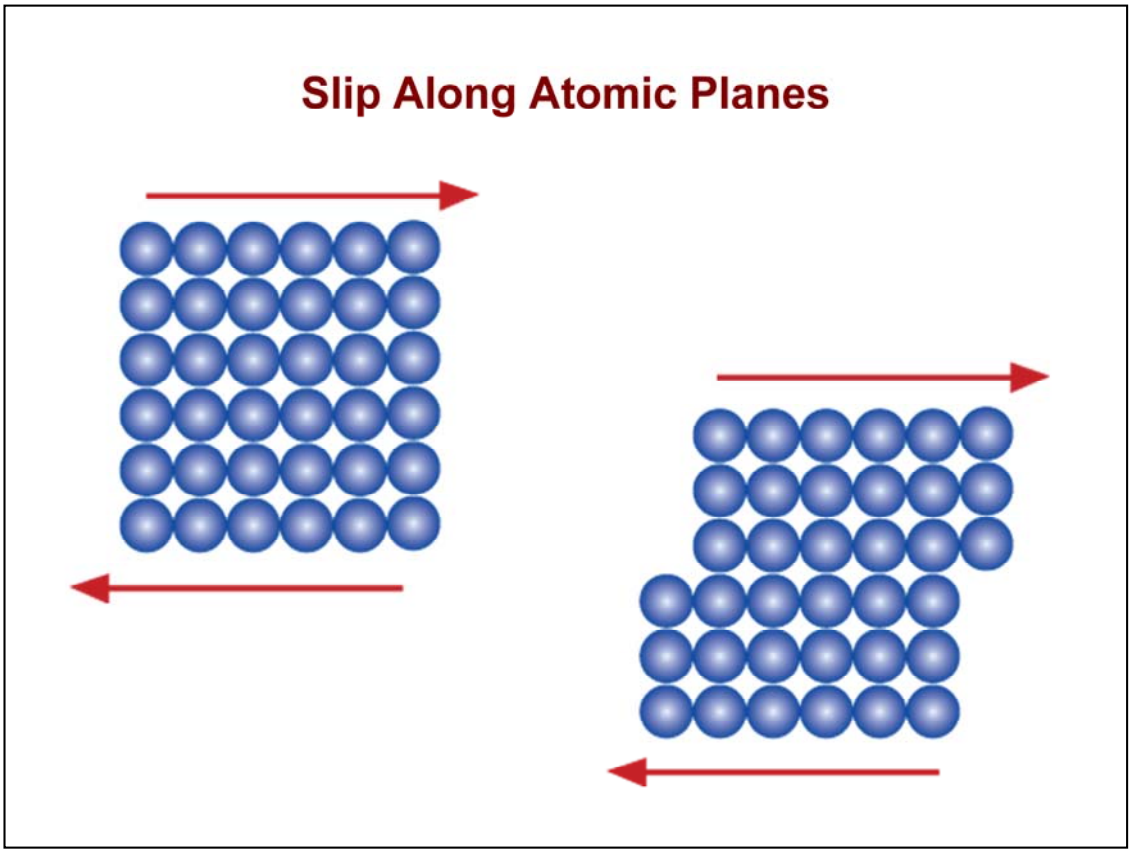
(Large) Atomic Movements

- In an ideal crystal, movement of atoms is very difficult because of the high energy barriers to motion through the lattice; defects provide low energy paths for the atomic movement.
- Defects are also responsible for the mobility of atoms under various external stimuli.
- Atomic movement can occur through slip along atomic planes, dislocation movement and diffusion.

Young

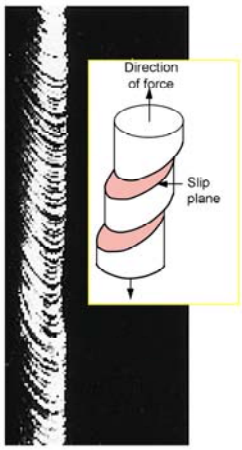
Slip Along Atomic Planes

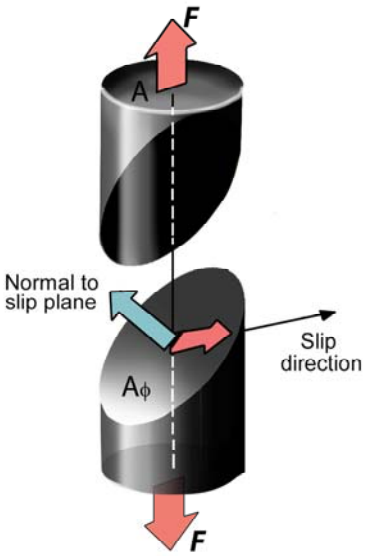
- Plastic deformation (i.e., deformation that remains after the load is removed) of metals occurs due to slip along atomic planes.
- The extent of the slip will depend on:
  - The magnitude and direction of shear stress
  - The bonding between the atomic planes
- In crystals, slip occurs along planes on which the atoms are most closely packed.


Slip Along Atomic Planes

Slip Along Atomic Planes

HCP Zinc

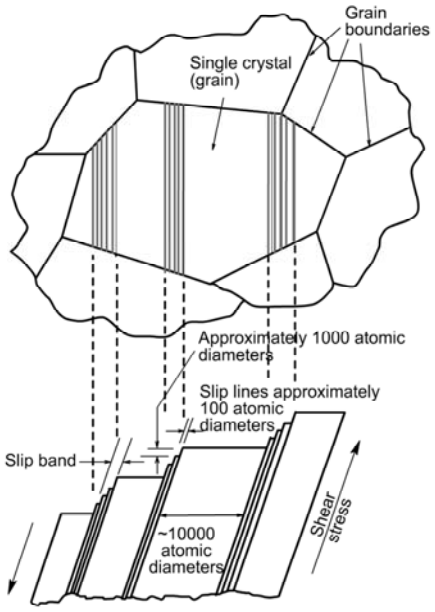




Slip is on planes ~45° to the applied tensile stress.

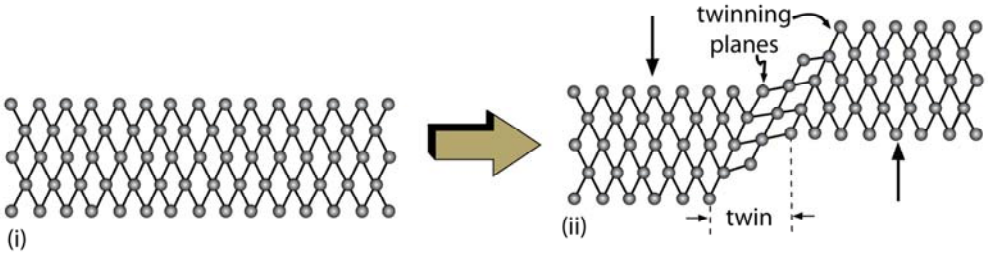
Slip Along Atomic Planes

Slip in a single crystal commences on the most favourably oriented slip system when the shear stress along the corresponding plane reaches some critical value.



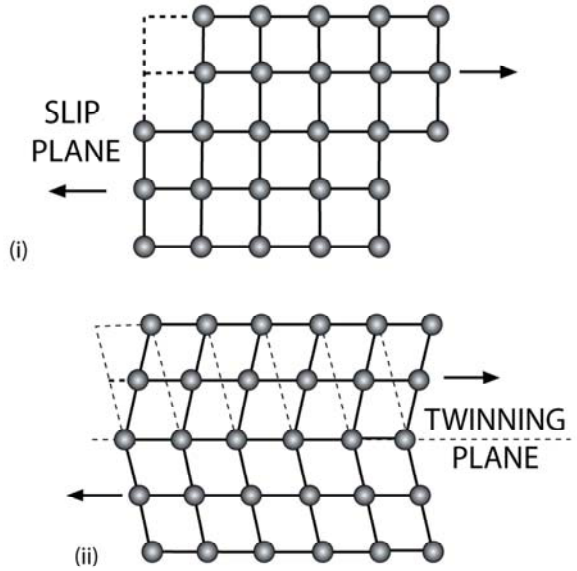
Deformation by Twinning

The stress required to produce twinning tends to be higher than that required to produce slip.



Deformation by twinning (due to stress)

Deformation by Twinning

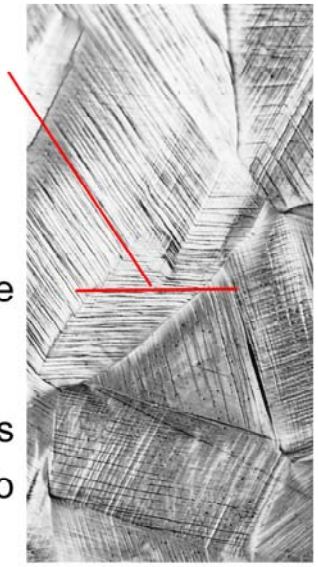


Difference between (i) slip and (ii) twinning

Higgins, Callister

Slip in Polycrystalline Solids

Slip lines on surface of polycrystalline Cu

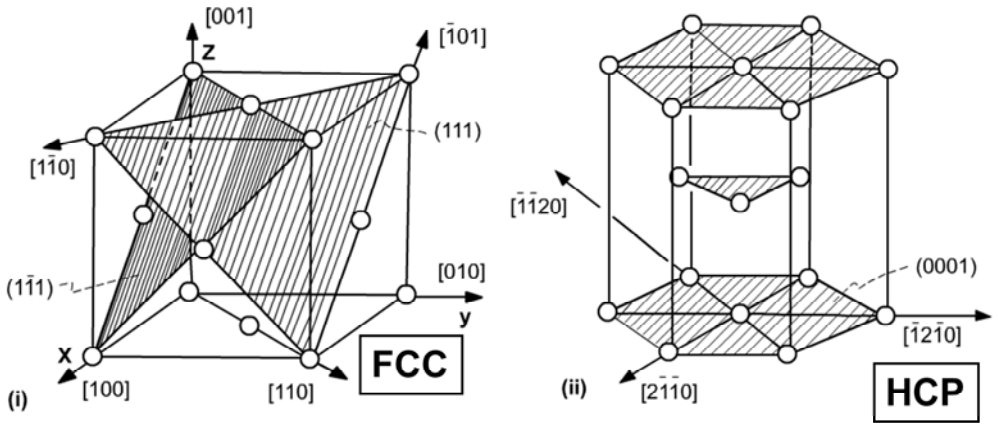


Slip planes and directions change from one crystal to another.

Materials with crystal structures having more slip systems undergo plastic deformation more easily.

Slip in Polycrystalline Solids

For example, Aluminium and Copper, with the FCC structure (2×6=12 planes) are more malleable and ductile than zinc, which has a HCP structure (3 parallel planes).



Young, Callister

Dislocation Movement

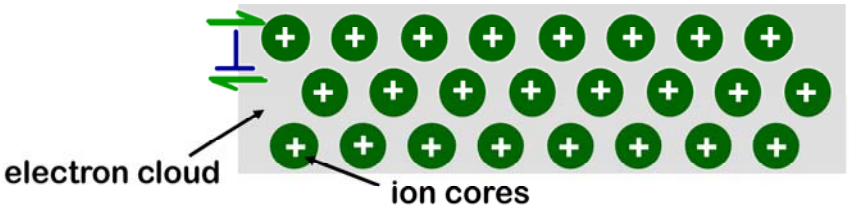
- Atomic movements are significantly easier in the vicinity of dislocations.
- Slip can occur by the movement of the dislocation; only a few atoms are involved in the slip. The net result is a shear deformation known as the Burgers vector.

Dislocation Movement

Metals: Dislocation motion is easier

-non-directional bonding

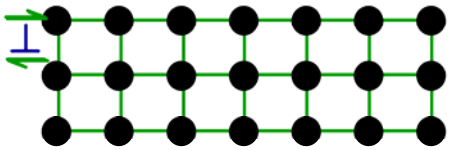
-close-packed planes for slip



Dislocation Movement

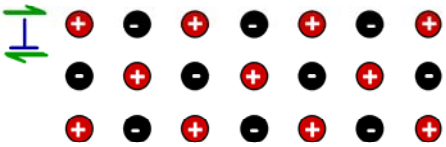
Covalent solids: Motion difficult

-directional (angular) bonding



Ionic solids: Motion difficult

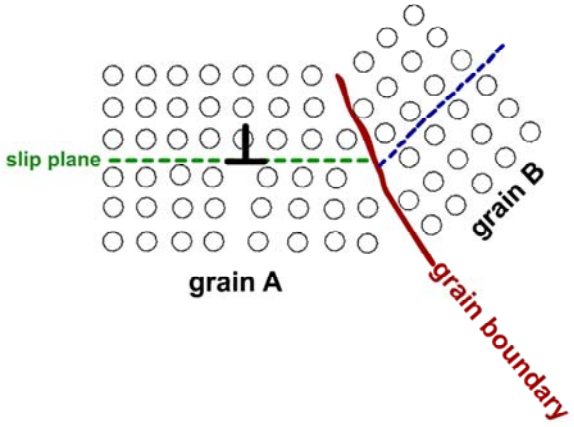
-need to avoid neighbors with same charge



M. Santhanam

Dislocation Movement

- Grain boundaries are barriers to slip.
- Barrier "strength" increases with misorientation.
- Smaller grain size: more barriers to slip.

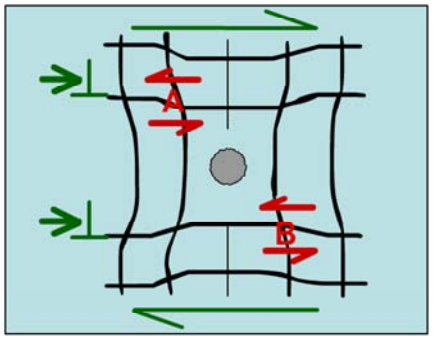


M. Santhanam

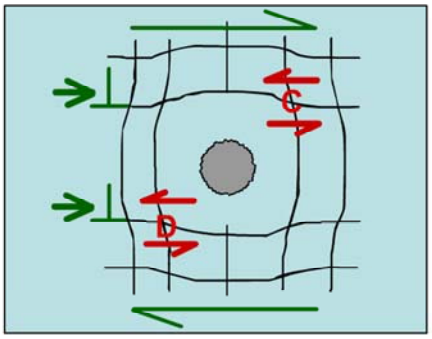
Dislocation Movement

- Impurity atoms distort the lattice & generate local strain.
- This becomes a barrier to dislocation motion.

Smaller substitutional impurity



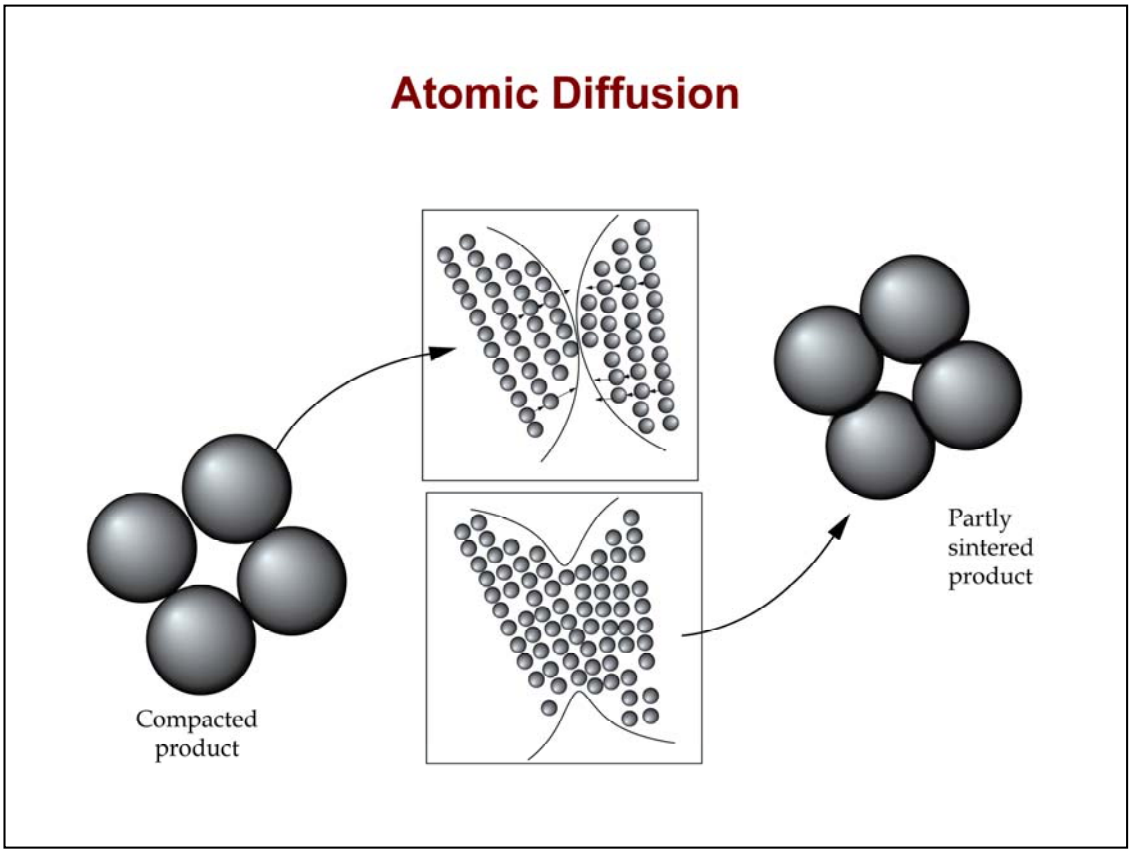
Larger substitutional impurity



M. Santhanam

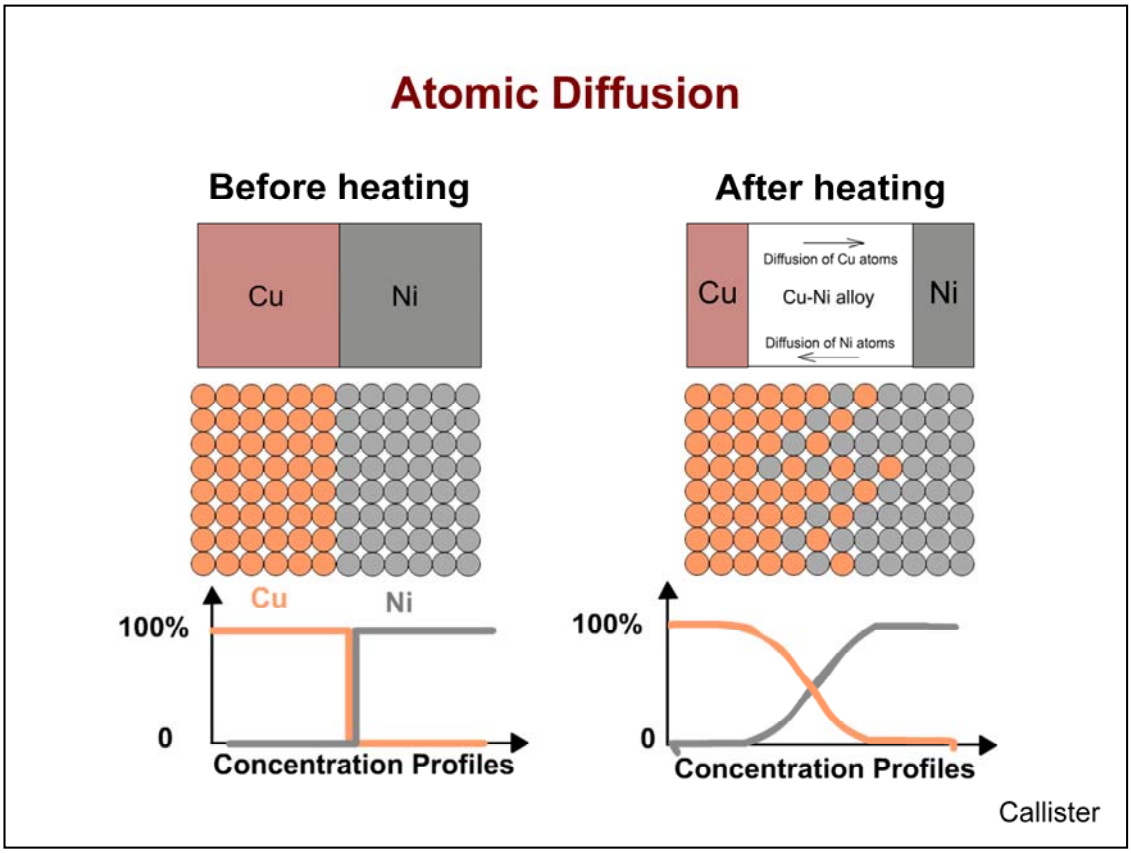
Atomic Diffusion

Many reactions and processes rely on the transfer of mass either within a specific solid or from a liquid, a gas or another solid phase. This is accomplished by diffusion, the phenomenon of material transport by atomic motion.


Atomic Diffusion
Compacted product
Partly sintered product

Atomic Diffusion

- *Diffusion couple* – Joining of bars of two different metals with close contact between the faces.
- This is called interdiffusion (or impurity diffusion), when one material diffuses into another.

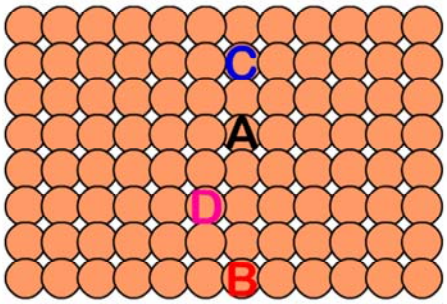

Atomic Diffusion
Before heating
After heating
Cu
Ni
Diffusion of Cu atoms
Cu-Ni alloy
Diffusion of Ni atoms
100%
0
Concentration Profiles
Callister

Atomic Diffusion

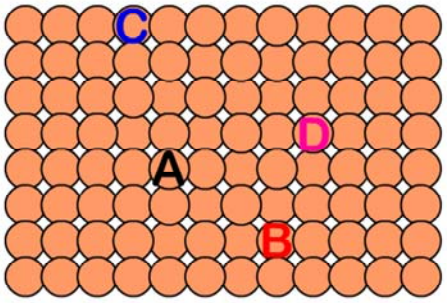
- The couple is heated for an extended period of time and then cooled.
- Before heating, the concentrations of Cu and Ni are uniform within the respective bar.
- Heating produces an alloyed diffusion zone with the concentrations of Cu and Ni as a function of position across the couple.

Atomic Diffusion

In pure metals, self-diffusion can occur where all the atoms exchanging positions are of the same type.



Label some atoms



After some time

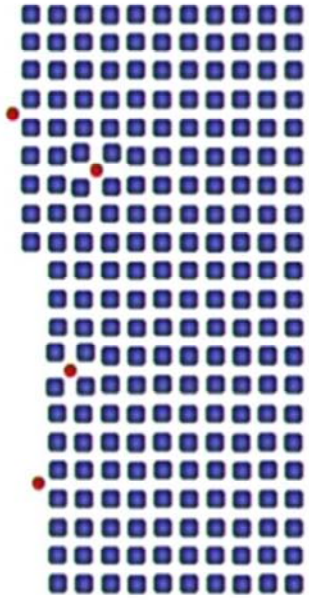
Diffusion Mechanisms

- Diffusion is the stepwise migration of atoms from lattice site to lattice site.

- For an atom to move, two conditions have to be met:
  - There must be an empty adjacent site
  - The atom must have sufficient energy to break bonds with its neighbour atoms, and then cause some lattice distortion during the displacement.

Diffusion Mechanisms

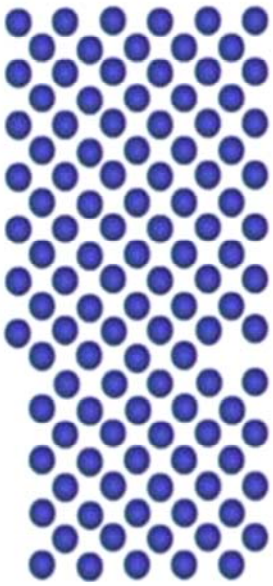
Interstitial diffusion involves atoms that migrate from an interstitial position to a neighbouring one that is empty. This mechanism is found for interdiffusion of impurities (H, C, N & O), which have atoms that are small enough to fit into the interstitial positions.



Interstitial diffusion

Callister

Diffusion Mechanisms

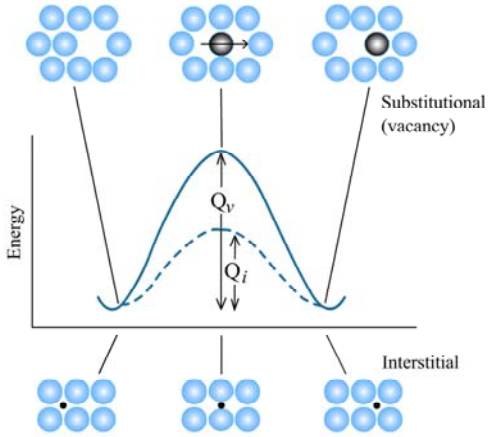


Vacancy diffusion involves the interchange of an atom from a normal lattice position to an adjacent vacant lattice site. This necessitates the presence of point defects in the form of vacancies.

Vacancy diffusion

Callister

Diffusion Mechanisms

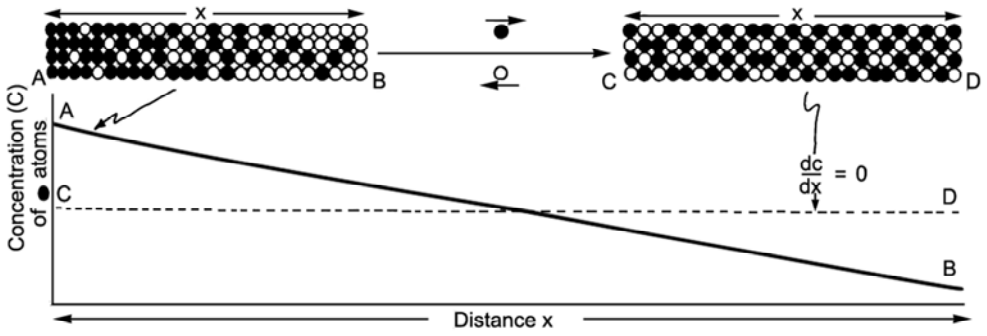


When an atom diffuses through the crystal lattice, it must move from its equilibrium position through a point where there are strong repulsive forces from its nearest neighbours. In addition, the lattice will be distorted.

This causes an energy barrier to the movement that must be overcome for diffusion to occur.

Q = Activation energy

Diffusion: *Fick´s Law*



AB is the initial concentration gradient, and CD is the final gradient after a long time during which diffusion was in progress

Higgins

Diffusion: *Fick´s Law*

The amount (J) of material moving across a unit area of a plane in unit time is proportional to the concentration gradient (dc/dx) at the same instant but of opposite sign:

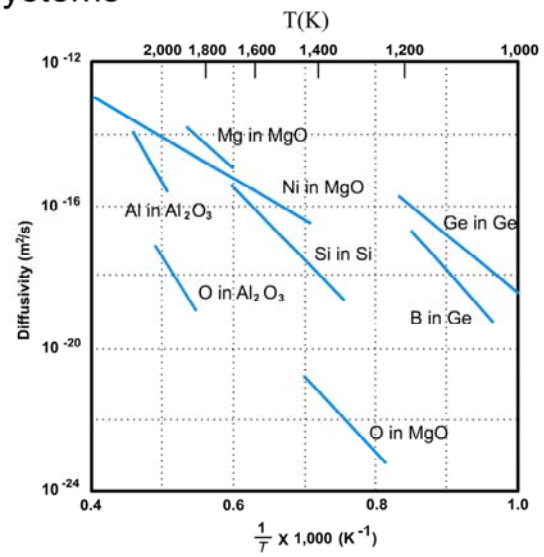
$$J = -D\frac{dc}{dx}$$

where D is the diffusion coefficient, and the x-axis is in the direction in which the concentration is acting. D is expressed in [m^2/s] units.

Diffusion Coefficient

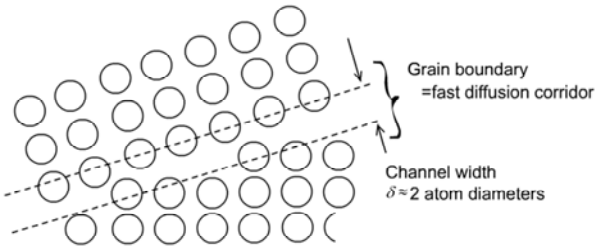
- The diffusion coefficient (or diffusivity) varies with:
  - Different solid solution systems
  - Temperature

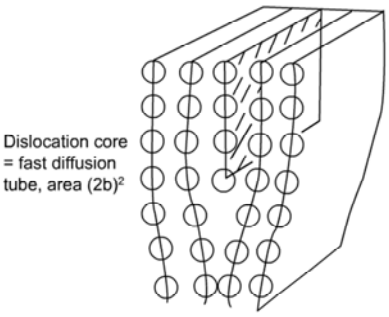
Diffusion also depends on the crystal structure. For example, diffusion is faster in BCC-Fe than in FCC-Fe (at the same temperature, e.g., 910°C) because the BCC structure is less closely-packed.



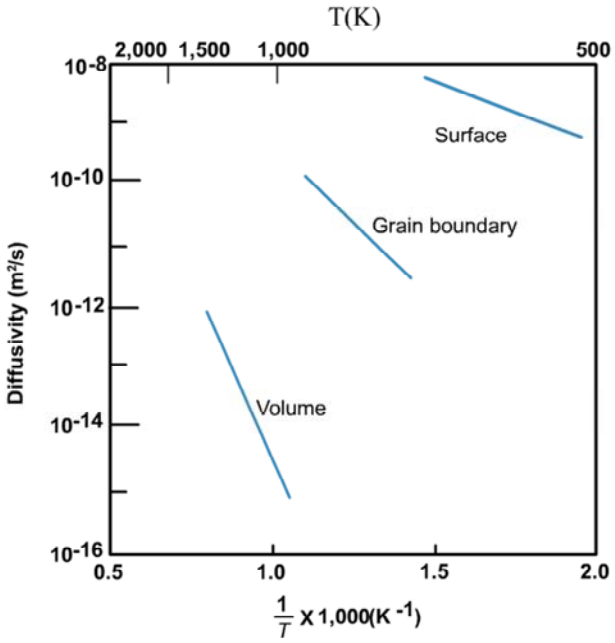
Fast Diffusion Paths

- Diffusion paths are faster through grain boundaries and dislocation cores.
- The grain boundary acts as a two atom wide planar channel, with a local diffusion rate that can be as much as 10^6 times greater than in the bulk.
- The dislocation core acts as a two atom wide high-conductivity tube.





Fast Diffusion Paths



Ashby & Jones

References

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