Imperfections, Defects and Diffusion

Lattice Defects

Types of Defects

- **Point defects** *(composition)*
  - Vacancies *(missing atoms)*
  - Interstitials *(extra atoms)*
  - Impurities *(unwelcome segregation)*

- **Extensive chemical changes**
  - Solid solutions
  - Not a defect in intentional alloying or doping

- **Line defects** *(1-dimensional)* *(Deformation)*
  - dislocations - in metals
Types of Defects, cont.

- Interfacial defects (2-dimensional) (Properties)
  - surfaces - both interior (pore walls) and exterior (surface of material)
  - interfaces -(grain boundaries)

- Bulk-Volume defects (3-dimensional)
  - cracks, foreign inclusions, other phases (including pores).

Point Defects in Metals

- Self Interstitial
- Substitutional Impurity
- Interstitial Impurity
- Vacancy
- Substitutional Impurity
Point defects

- **Vacancy**
  - An empty atomic site

- **Interstitial**
  - An atom somewhere other than an atomic site
    - Self-interstitial
    - Impurity interstitial

- **Substitutional impurity**
  - Some “foreign” species on an atomic site

**Line Defects: Dislocation in Metals**

- Linear (one dimensional) defect around which some of the atoms are misaligned

Responsible for large mechanical deformation in crystalline solids

*Edge Dislocation*
Types of Dislocations

- **Edge Dislocation:**
  A portion of an extra plane of atoms

- **Screw Dislocation:**
  Helical atomic displacement around a line extending through the crystal

- **Mixed Dislocation:**
  Some edge, some screw nature

Edge Dislocation
Burgers vector

Perfect crystal

\( b \)

dislocated crystal

\( b \)-represents the magnitude of the structural defect

Screw Dislocation

Dislocation line

Burgers vector, \( b \)
Mixed Dislocation

Why are Dislocations Important?

The motion of dislocations is the principle mechanism whereby metals deform.

- Lower energy than breaking all bonds in a plane at once

Shear occurs by dislocation movement producing permanent (plastic) deformation by “slip”

Textbook ch6, pp 212-218

Slip plane

Direction of dislocation movement

(a) (b) (c)
Edge Dislocation Motion - 3D

Slip occurs along densely packed directions on densely packed planes
(Plane)[Direction] pairs designate “slip systems” (e.g., in FCC and HCP) on page 215.

Dislocation movement and ductility

- A large number of independent slip systems are required for good ductility in polycrystalline materials so grains can deform to accommodate their neighboring grains. Common in many metal structures (bcc and fcc).

- Dislocations are very complex in ceramic structures. This and complications of like charged ions encountering each other during slip make dislocation movement almost impossible in ceramics. Therefore ceramics are not ductile, they are brittle.
Impediments to easy dislocation movement

- Impurity atoms ("solute hardening")
- Intersection with other dislocations (entanglement) ("work hardening")
- Grain boundaries (dislocations "pile up")
- Small dispersed inclusions ("precipitation hardening")
- All of these affect ductility and yield strength of a metals

Grain boundaries and other dislocations impede the movement of dislocations causing "hardening"
Material Science Investigative Techniques “Microscopy”

- Optical microscope
  surface microstructure (~1 µm)

- Scanning electron microscope (SEM)
  Surface microstructure, analytical chemistry (~50-100 nm)

- Transmission electron microscope
  resolve the atomic structure from a very thin foil (30 Å), (~1 Å)

- Atomic force microscope
  3D surface topography, electrical, magnetic scanning (~1 nm)

Reading Assignment

Shackelford 2001(5th Ed)
- Read Chapter 4, pp 115-136, 145-150
  Read ahead Chapter 5, pp 158-181