CHAPTER 4:
IMPERFECTIONS IN SOLIDS

ISSUES TO ADDRESS...

- What types of defects arise in solids?
- Can the number and type of defects be varied and controlled?
- How do defects affect material properties?
- Are defects undesirable?
TYPES OF IMPERFECTIONS

- Vacancy atoms
- Interstitial atoms
- Substitutional atoms  Point defects

- Dislocations  Line defects
- Grain Boundaries  Area defects
POINT DEFECTS

- **Vacancies**: vacant atomic sites in a structure.

- **Self-Interstitionals**: "extra" atoms positioned between atomic sites.
- Equilibrium concentration varies with temperature!

\[ \frac{N_D}{N} = \exp \left( \frac{-Q_D}{kT} \right) \]

- No. of defects
- No. of potential defect sites.
- Boltzmann's constant
  - (1.38 x 10^{-23} J/atom K)
  - (8.62 x 10^{-5} eV/atom K)
- Each lattice site is a potential vacancy site
MEASURING ACTIVATION ENERGY

- We can get $Q$ from an experiment.
- Measure this...

\[
\frac{N_D}{N} = \exp\left(\frac{-Q_D}{kT}\right)
\]

- Replot it...

\[\ln\frac{N_D}{N} = \frac{1}{T}\]

slope $\frac{-Q_D}{k}$

defect concentration

Exponential dependence!
ESTIMATING VACANCY CONC.

• Find the equil. # of vacancies in 1 m$^3$ of Cu at 1000°C.

$\rho = 8.4 \text{ g/cm}^3$  \hspace{1cm} $ACu = 63.5\text{ g/mol}$

$Q_V = 0.9\text{ eV/atom}$  \hspace{1cm} $NA = 6.02 \times 10^{23} \text{ atoms/mole}$

$$\frac{N_D}{N} = \exp\left(-\frac{Q_D}{kT}\right) = 2.7 \cdot 10^{-4}$$

For 1m$^3$, $N = \rho \times \frac{NA}{ACu} \times 1m^3 = 8.0 \times 10^{28} \text{ sites}$

• Answer:

$N_D = 2.7 \cdot 10^{-4} \cdot 8.0 \times 10^{28} \text{ sites} = 2.2x 10^{25} \text{ vacancies}$
POINT DEFECTS IN ALLOYS

Two outcomes if impurity (B) added to host (A):

- **Solid solution** of B in A (i.e., random dist. of point defects)
  
  ![Substitutional alloy](image)
  
  **Substitutional** alloy
  (e.g., Cu in Ni)

  ![Interstitial alloy](image)
  
  **Interstitial** alloy
  (e.g., C in Fe)

- Solid solution of B in A plus particles of a new phase (usually for a larger amount of B)
  
  ![Second phase particle](image)
  
  Second phase particle
  --different **composition**
  --often different structure.
**Alloy Composition**

**Weight Percentage**

**Binary**  
(2 components)  
\[ C_1 = \frac{m_1}{m_1 + m_2} \times 100 \]

**Atomic or Mole Percentage**

\[ C_1' = \frac{n_{m1}}{n_{m1} + n_{m2}} \times 100 \]

\[ n_{m1} = \frac{m_1}{A_1} \]

**Ternary, Quaternary, …**  
(3, 4, … components)  
\[ C_j = \frac{m_j}{\sum_i m_i} \times 100 \]

\[ C_j' = \frac{n_{mj}}{\sum_i n_{mi}} \times 100 \]

**Conversion formulas**

\[ C_1' = \frac{C_1 A_2}{C_1 A_2 + C_2 A_1} \times 100 \]

\[ C_1 = \frac{C_1' A_1}{C_1' A_1 + C_2' A_2} \times 100 \]
Dislocations

Line defects

Most important class of defects for ductile crystalline materials (metals!)

Burgers vector $\mathbf{b}$
Basic lattice deformation

Edge Dislocations
$\mathbf{b}$ perpendicular to the dislocation line

Schematic atomic structure of an edge dislocation
Screw Dislocations

Schematic perspective view

View of plane ABCD

Screw dislocation line

Burgers vector $\mathbf{b}$
Basic lattice deformation

Screw Dislocations
$\mathbf{b}$ parallel to the dislocation line
Mixed Dislocations

Schematic perspective view

Schematic of dislocation line

View of plane ABCD
Images of Dislocations

Dislocations in Ti alloy
Dislocations in GaN
Interfacial Defects

Two-dimensional defects – also referred to as planar defects

Free surfaces
Surfaces are ‘defects’ – typical energies $0.1 – 1 \text{ J/cm}^2$

Grain Boundaries
Borders between crystals with different orientation

High angle grain boundary
Large misorientation

Low-angle grain boundary
Small misorientation
Consists of walls of dislocations
Low Angle Grain Boundaries

Example of a tilt boundary

Grain 1

Grain Boundary

Grain 2

Low angle boundaries

\[ \theta \approx \frac{b}{d} \]

\( \theta = \) Grain-Grain misorientation

\( b = \) Burgers vector

\( d = \) dislocation spacing

Edge dislocations
Observation of Microstructures

Optical Microscopy (referred to as metallography, ceramography, ...)

Resolution of optical microscopy \( \approx \lambda_{\text{light}} \approx 500 \, \text{nm} \)
Observation of Microstructures

Optical Microscope  Transmission Electron Microscope

FEI Tecnai F30
300 kV FE TEM/STEM (UCSB)

TEM/STEM Resolution
~ 1 Å
Observation of Microstructures

**Scanning Electron Microscope**

![Typical SEM Image](image)

**SEM Resolution**

\[ \sim 10 \, \text{Å} \]
Observation of Microstructures

Scanning Probe Microscopy (SPM)

Common modes
Scanning Tunneling Microscopy (STM)
Atomic Force Microscopy (AFM)

AFM Image: GaN

Figure 2-3. Typical optical detection scheme in AFM.

Figure 2-1. SPM feedback loop.

SPM Resolution: ~ 1 Å
CHAPTER 6: MECHANICAL PROPERTIES

ISSUES TO ADDRESS...

• **Stress** and **strain**: What are they and why are they used instead of load and deformation?

• **Elastic** behavior: When loads are small, how much deformation occurs? What materials deform least?

• **Plastic** behavior: At what point do dislocations cause permanent deformation? What materials are most resistant to permanent deformation?

• **Toughness** and **ductility**: What are they and how do we measure them?
ELASTIC DEFORMATION

1. Initial

2. Small load
   - Bonds stretch

3. Unload
   - Return to initial

Elastic means reversible!
PLASTIC DEFORMATION (METALS)

1. Initial
2. Small load
   - bonds stretch & planes shear
3. Unload
   - planes still sheared

Plastic means **permanent**!

**F**

δ_{elastic + plastic}

δ_{plastic}

linear elastic

δ_{plastic}

linear elastic
ENGINEERING STRESS

- **Tensile stress, \( \sigma \):**
  \[
  \sigma = \frac{F_t}{A_o}
  \]
  
  Stress has units: \( \text{N/m}^2 \) or \( \text{lb/in}^2 \)

- **Shear stress, \( \tau \):**
  \[
  \tau = \frac{F_s}{A_o}
  \]
COMMON STATES OF STRESS

• **Simple tension**: cable

\[ \sigma = \frac{F}{A_o} \]

\( A_o \) = cross sectional Area (when unloaded)

\[ \sigma = \frac{F}{A_o} \]

Note: \( \tau = \frac{M}{A_c R} \) here.

• **Simple shear**: drive shaft

\[ \tau = \frac{F_S}{A_o} \]

\( F_S \) = applied shear force

\( A_o \) = cross sectional area

\( A_c \) = moment of inertia

\( 2R \) = radius of gyration

\( M \) = applied moment

\( \tau \) = shear stress

Ski lift (photo courtesy P.M. Anderson)
**OTHER COMMON STRESS STATES (1)**

- **Simple compression:**

  - **Balanced Rock, Arches National Park**
    (photo courtesy P.M. Anderson)

  - **Canyon Bridge, Los Alamos, NM**
    (photo courtesy P.M. Anderson)

  \[
  \sigma = \frac{F}{A_0}
  \]

  Note: compressive structure member \((\sigma < 0 \text{ here})\).
OTHER COMMON STRESS STATES (2)

- **Bi-axial tension:**
  - Pressurized tank (photo courtesy P.M. Anderson)
  - $\sigma_\theta > 0$
  - $\sigma_z > 0$

- **Hydrostatic compression:**
  - Fish under water (photo courtesy P.M. Anderson)
  - $\sigma_h < 0$
ENGINEERING STRAIN

- **Tensile strain:**
  \[ \varepsilon = \frac{\delta}{L_0} \]

- **Lateral strain:**
  \[ \varepsilon_L = -\frac{\delta_L}{W_0} \]

- **Shear strain:**
  \[ \gamma = \tan \theta \]

Strain is always dimensionless.
STRESS-STRAIN TESTING

• Typical tensile specimen

• Other types of tests:
  -- compression: brittle materials (e.g., concrete)
  -- torsion: cylindrical tubes, shafts.

Adapted from Fig. 6.2, *Callister 6e.*

Adapted from Fig. 6.3, *Callister 6e.*
LINEAR ELASTIC PROPERTIES

• **Modulus of Elasticity, \( E \):** (also known as Young's modulus)

• **Hooke's Law:**
  \[
  \sigma = E \varepsilon
  \]

• **Poisson's ratio, \( \nu \):**
  \[
  \nu = -\frac{\varepsilon_L}{\varepsilon}
  \]

  - metals: \( \nu \sim 0.33 \)
  - ceramics: \( \sim 0.25 \)
  - polymers: \( \sim 0.40 \)

**Units:**

- \( E \): [GPa] or [psi]
- \( \nu \): dimensionless

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![Diagram showing linear elastic behavior with modulus of elasticity and Poisson's ratio](image-url)
OTHER ELASTIC PROPERTIES

- Elastic Shear modulus, $G$:
  \[ \tau = G \gamma \]

- Elastic Bulk modulus, $K$:
  \[ P = -K \frac{\Delta V}{V_0} \]

- Special relations for isotropic materials:
  \[ G = \frac{E}{2(1 + \nu)} \quad K = \frac{E}{3(1 - 2\nu)} \]
YOUNG’S MODULI: COMPARISON

Based on data in Table B2, Callister 6e. Composite data based on reinforced epoxy with 60 vol% of aligned carbon (CFRE), aramid (AFRE), or glass (GFRE) fibers.