

# Materials Engineering

## Lattice Parameters

SC :  $a = 2R$

BCC :  $a\sqrt{3} = 4R$

FCC :  $a\sqrt{2} = 4R$

DC :  $a = \frac{8R}{\sqrt{3}}$

## Points, Directions and Planes Notation

Points :  $x, y, z$

Direction (singular) :  $[h \ k \ l]$

Direction (family) :  $\langle h \ k \ l \rangle$

Planes (singular) :  $(h \ k \ l)$

Planes (family) :  $\{h \ k \ l\}$

## Density (metals)

$$\rho = \frac{nA}{V_c N_A}$$

## %Ionic Character

$$\% \text{IC} = [1 - \exp\{-(0.25)(X_A - X_B)^2\}] \times 100$$

## Linear Density

$$LD = \frac{L_{\text{occupied}}}{L_{\text{total}}}$$

## Planar Density

$$PD = \frac{A_{\text{occupied}}}{A_{\text{total}}}$$

## Atomic Packing Factor

$$APF = \frac{V_{\text{occupied}}}{V_{\text{total}}}$$

## Bragg's Law

$$n\lambda = 2d_{hkl} \sin \theta$$

## Inter-Planar Spacing (for cubic symmetries)

$$d_{hkl} = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$$

## Vacancies/Unit Volume

$$N_v = N \exp\left(-\frac{Q_v}{kT}\right)$$

## Atomic Sites/Unit Volume

$$N = \frac{N_A \rho}{A}$$

## Composition (weight %)

$$C_w = \frac{m_1}{m_1 + m_2} \times 100$$

## Composition (atomic %)

$$C_a = \frac{n_{m1}}{n_{m1} + n_{m2}} \times 100$$

## Mean Intercept Length

$$\bar{l} = \frac{L_T}{PM}$$

# Diffusion

## Diffusion Flux

$$J = \frac{M}{At}$$

## Fick's First Law

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

## Fick's Second Law

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

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

## Temperature Dependence of Diffusion Coefficient

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

# Mechanical Properties

## Engineering Stress

$$\sigma = \frac{F}{A_0}$$

## Engineering Strain

$$\epsilon = \frac{l_i - l_0}{l_0} = \frac{\Delta l}{l_0}$$

## Hooke's Law

$$\sigma = E\epsilon$$

## Poisson's Ratio

$$\nu = -\frac{\epsilon_x}{\epsilon_z} = \frac{\epsilon_y}{\epsilon_z}$$

## Ductility % Elongation

$$\%EL = \left(\frac{l_f - l_0}{l_0}\right) \times 100$$

## Ductility % Area Reduction

$$\%RA = \left(\frac{A_0 - A_f}{A_0}\right) \times 100$$

### True Stress

$$\sigma_T = \frac{F}{A_i}$$

### True Strain

$$\epsilon_T = \ln \frac{l_i}{l_0}$$

### Plastic Region to the Point of Necking

$$\sigma_T = K \epsilon_T^n$$

### Resolved Shear Stress

$$\tau_R = \sigma \cos \phi \cos \lambda$$

### Critical Resolved Shear Stress

$$\tau_{crss} = \sigma_y (\cos \phi \cos \lambda)_{max}$$

### Hall-Petch Equation

$$\sigma_y = \sigma_0 + k_y d^{-1/2}$$

### Percent Cold Work

$$\% CW = \left( \frac{A_0 - A_d}{A_0} \right) \times 100$$

### Average Grain Size

$$d^n - d_0^n = Kt$$

→ During grain growth

## Failure/Fracture Mechanics

### Elliptical Cracks

$$\sigma_m = 2\sigma_0 \left( \frac{a}{p_t} \right)^{1/2}$$

→ Where 'a' is the length of an edge external crack, and '2a' is the length of an internal crack.

### Fracture Toughness

$$K_c = Y\sigma_c \sqrt{\pi a}$$

### Critical Stress

$$\sigma_c = \frac{K_{Ic}}{Y\sqrt{\pi a}}$$

### Maximum Flaw Size

$$a_c = \frac{1}{\pi} \left( \frac{K_{Ic}}{\sigma Y} \right)^2$$

### Mean Stress (fatigue tests)

$$\sigma_m = \frac{\sigma_{max} + \sigma_{min}}{2}$$

### Stress Amplitude (fatigue tests)

$$\sigma_a = \frac{\sigma_{max} - \sigma_{min}}{2}$$

### Range of Stress (fatigue tests)

$$\sigma_r = \sigma_{max} - \sigma_{min}$$

### Max. Stress for Fatigue

### Rotating-Bending Tests

$$\sigma = \frac{16FL}{\pi d_0^3}$$

### Thermal Stress

$$\sigma = \alpha_l E \Delta T$$

### Steady-State Creep Rate

$$\dot{\epsilon}_s = K_1 \sigma^n \text{ (constant T)}$$

$$\dot{\epsilon}_s = K_2 \sigma^n \exp \left( -\frac{Q_c}{RT} \right)$$

### Larson-Miller Parameter

$$m = T(C + \log t_r)$$

## Phase Diagrams

### Mass Fraction - Liquid Phase

$$W_L = \frac{C_\alpha - C_0}{C_\alpha - C_L}$$

→ For binary isomorphous

### Mass Fraction - Solid Phase

$$W_\alpha = \frac{C_0 - C_L}{C_\alpha - C_L}$$

→ For binary isomorphous

## Phase Transformations

### Critical Radius for Stable Solid Particle

$$r^* = \left( -\frac{2\gamma T_m}{\Delta H_f} \right) \left( \frac{1}{T_m - T} \right)$$

Homogenous nucleation:

$$r^* = -\frac{2\gamma}{\Delta G_v}$$

Heterogenous nucleation:

$$r^* = -\frac{2\gamma_{SL}}{\Delta G_v}$$

### Activation Free Energy for Formation of Stable Solid Particle

$$\Delta G^* = \left( \frac{16\pi\gamma^3 T_m^2}{3\Delta H_f^2} \right) \frac{1}{(T_m - T)^2}$$

Homogenous nucleation:

$$\Delta G^* = \frac{16\pi\gamma^3}{3(\Delta G_v)^2}$$

Heterogenous nucleation:

$$\Delta G^* = \left( \frac{16\pi\gamma_{SL}^3}{3(\Delta G_v)^2} \right) S(\theta)$$

## Interfacial Energies with Heterogenous Nucleation

$$\gamma_{IL} = \gamma_{SI} + \gamma_{SL} \cos \theta$$

## Fraction of Transformation

$$y = 1 - \exp(-kt^n)$$

## Transformation Rate

$$\text{rate} = \frac{1}{t_{0.5}}$$

## Ceramic Properties

### Density (Ceramics)

$$\rho = \frac{n'(\sum A_C + \sum A_A)}{V_C N_A}$$

### Flexural Strength

Rectangular cross section:

$$\sigma_{fs} = \frac{3F_f L}{2bd^2}$$

$$\epsilon = \frac{6 \cdot d \cdot \Delta y}{L^2}$$

Circular cross section:

$$\sigma_{fs} = \frac{F_f L}{\pi R^3}$$

$$\epsilon = \frac{12 \cdot R \cdot \Delta y}{L^2}$$

### Porous Ceramics

Elastic modulus:

$$E = E_0(1 - 1.9P + 0.9P^2)$$

Flexural strength:

$$\sigma_{fs} = \sigma_0 \exp(-nP)$$

## Polymer Properties

### Molecular Weight

Number-Average:

$$\bar{M}_n = \sum x_i M_i$$

Weight-Average:

$$\bar{M}_w = \sum w_i M_i$$

For copolymers, average repeat unit molecular weight:

$$\bar{m} = \sum f_i m_i$$

### Degree of Polymerization

$$n = \frac{\bar{M}_n}{m}$$

### % Crystallinity by Weight

$$\% C = \frac{\rho_c(\rho_s - \rho_a)}{\rho_s(\rho_c - \rho_a)} \times 100$$

### Diffusion Flux

$$J = -P_M \frac{\Delta P}{\Delta x}$$

→ For steady state diffusion through a polymer membrane

### Relaxation Modulus

$$E_r(t) = \frac{\sigma(t)}{\epsilon_0}$$

### Polymer Tensile Strength

$$TS = TS_\infty - \frac{A}{\bar{M}_n}$$

## Composites

### Rules of Mixtures

Transverse properties:

$$E_c^{trans} = \frac{E_m E_f}{E_m V_f + E_f V_m}$$

Axial/longitudinal properties:

$$E_c^{long} = E_m V_m + E_p V_p$$

### Critical Fiber Length

$$l_c = \frac{\sigma_f^* d}{2\tau_c}$$

### Longitudinal Tensile Strength

For continuous and aligned fibrous composite:

$$\sigma_{cl}^* = \sigma_m'(1 - V_f) + \sigma_f^* V_f$$

For discontinuous and aligned fibrous composite and  $l > l_c$ :

$$\sigma_{cd}^* = \sigma_f^* V_f \left(1 - \frac{l_c}{2l}\right) + \sigma_m'(1 - V_f)$$

For discontinuous and aligned fibrous composite and  $l < l_c$ :

$$\sigma_{cd'}^* = \frac{l\tau_c}{d} V_f + \sigma_m'(1 - V_f)$$

## Corrosion and Degradation

### Electrochemical Cell Potential

For two standard half-cells:

$$\Delta V^0 = V_2^0 - V_1^0$$

For two nonstandard half-cells:

$$\Delta V = (V_2^0 - V_1^0) - \frac{RT}{n\mathcal{F}} \ln \frac{[M_1^{n+}]}{[M_2^{n+}]}$$

For two nonstandard half-cells, room temperature:

$$\Delta V = (V_2^0 - V_1^0) - \frac{0.0592}{n} \log \frac{[M_1^{n+}]}{[M_2^{n+}]}$$

### Corrosion Penetration Rate

$$\text{CPR} = \frac{KW}{\rho A t}$$

### Corrosion Rate

$$r = \frac{i}{n\mathcal{F}}$$

### Overvoltage

For activation polarization:

$$\eta_a = \pm \beta \log \frac{i}{i_0}$$

For concentration polarization:

$$\eta_c = \frac{2.3RT}{n\mathcal{F}} \log \left( 1 - \frac{i}{i_L} \right)$$

### Pilling-Bedworth Ratio

For divalent metals:

$$\text{P-B ratio} = \frac{A_o \rho_M}{A_M \rho_o}$$

For other than divalent metals:

$$\text{P-B ratio} = \frac{A_o \rho_M}{a A_M \rho_o}$$

### Metal Oxidation

Parabolic rate expression:

$$W^2 = K_1 t + K_2$$

Linear rate expression:

$$W = K_3 t$$

Logarithmic rate expression:

$$W = K_4 \log(K_5 t + K_6)$$

## Electrical Properties

### Ohm's Law

$$V = IR$$

### Electrical Resistivity

$$\rho = \frac{RA}{l}$$

### Electrical Conductivity

$$\sigma = \frac{1}{\rho}$$

### Current Density

$$J = \sigma \mathcal{E}$$

### Electrical Field Intensity

$$\mathcal{E} = \frac{V}{l}$$

### (Metals) Conductivity for $n$ -Type Extrinsic Semiconductor

$$\sigma = n e \mu_e$$

### (Metals) Matthiessen's Rule

$$\rho_{total} = \rho_t + \rho_i + \rho_d$$

### Thermal Resistivity

#### Contribution

$$\rho_t = \rho_0 + aT$$

### Impurity Resistivity

#### Contribution

Impurity resistivity contribution, single-phase alloy:

$$\rho_i = A c_i (1 - c_i)$$

Impurity resistivity contribution, two-phase alloy:

$$\rho_i = \rho_\alpha V_\alpha + \rho_\beta V_\beta$$

### Conductivity for Intrinsic Semiconductor

$$\begin{aligned} \sigma &= n e \mu_e + p e \mu_h \\ &= n_i e (\mu_e + \mu_h) \end{aligned}$$

### Conductivity for $p$ -Type Extrinsic Semiconductor

$$\sigma \cong p e \mu_h$$

### Capacitance

$$C = \frac{Q}{V}$$

Parallel-plate capacitor (vacuum):

$$C = \epsilon_0 \frac{A}{l}$$

Parallel-plate capacitor (dielectric medium between plates):

$$C = \epsilon \frac{A}{l}$$

### Dielectric Constant

$$\epsilon_r = \frac{\epsilon}{\epsilon_0}$$

## Dielectric Displacement

$$D = \epsilon_0 \mathcal{E} + P$$

In a vacuum:

$$D_0 = \epsilon_0 \mathcal{E}$$

In a dielectric material:

$$D = \epsilon \mathcal{E}$$

## Polarization

$$P = \epsilon_0(\epsilon_r - 1)\mathcal{E}$$

## Thermal Properties

### Heat Capacity

$$C = \frac{dQ}{dT}$$

Linear Coefficient of

### Thermal Expansion

$$\frac{l_f - l_0}{l_0} = \alpha_l(T_f - T_0)$$

$$\frac{\Delta l}{l_0} = \alpha_l \Delta T$$

Volume Coefficient of

### Thermal Expansion

$$\frac{\Delta V}{V_0} = \alpha_v \Delta T$$

### Thermal Conductivity

$$q = -k \frac{dT}{dx}$$

### Thermal Stress

$$\sigma = E\alpha_l(T_0 - T_f)$$

$$= E\alpha_l \Delta T$$

## Thermal Shock Resistance

### Parameter

$$\text{TSR} \cong \frac{\sigma_f k}{E\alpha_l}$$

## Magnetic Properties

### Magnetic Field Strength - Coil

$$H = \frac{NI}{l}$$

### Magnetic Flux Density

$$B = \mu_0 H + \mu_0 M$$

In a material:

$$B = \mu H$$

In a vacuum:

$$B_0 = \mu_0 H$$

For a ferromagnetic material:

$$B \cong \mu_0 M$$

### Relative Permeability

$$\mu_r = \frac{\mu}{\mu_0}$$

### Magnetization

$$M = X_m H$$

### Magnetic Susceptibility

$$X_m = \mu_r - 1$$

### Saturation Magnetization

For Ni:

$$M_s = 0.60\mu_B N$$

For a ferrimagnetic material:

$$M_s = N' \mu_B$$

## Optical Properties

### Velocity of Light

In a vacuum:

$$c = \frac{1}{\sqrt{\epsilon_0 \mu_0}}$$

In a medium:

$$v = \frac{1}{\sqrt{\epsilon \mu}}$$

Velocity of

### Electromagnetic Radiation

$$c = \lambda \nu$$

### Index of Refraction

$$n = \frac{c}{v} = \sqrt{\epsilon_r \mu_r}$$

### Reflectivity

$$R = \left( \frac{n_2 - n_1}{n_2 + n_1} \right)^2$$

### Intensity of Transmitted Radiation

$$I'_T = I'_0 e^{-\beta x}$$

→ (Reflection losses not taken into account)

Intensity of Radiation

### Transmitted

$$I_T = I_0(1 - R)^2 e^{-\beta l}$$

→ (Reflection losses taken into account)

Many equations were referenced from *Callister, W. D. (2012).*

*Materials science and engineering: An introduction 8E. John Wiley & Sons.*