Materials Engineering

Lattice Paramaters

$$SC: a = 2R$$

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

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

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

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

% 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)

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

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

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

Ductility % Elongation

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

Ductility % Area Reduction

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

Materials

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

$$\sigma_{\rm v} = \sigma_0 + k_{\rm v} d^{-1/2}$$

Percent Cold Work

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

Average Grain Size

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

 \rightarrow 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

$$\sigma = \alpha_t E \Delta T$$

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

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

→ For binary isomorphous

Mass Fraction - Solid Phase

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

 \rightarrow For binary isomorphous

Phase Transformations

Critical Radius for Stable

Solid Particle

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

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:

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

Materials

Interfacial Energies with <u>Heterogenous Nucleation</u>

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

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

Transformation Rate

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

Ceramic Properties

Density (Ceramics)

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

Flexural Strength

Rectangular cross section:

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

Circular cross section:

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

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

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

Diffusion Flux

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

 \rightarrow 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

$$CPR = \frac{KW}{\rho At}$$

Corrosion Rate

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

Overvoltage

For activation polarization:

$$\eta_{\alpha} = \pm \beta \log \frac{i}{i_0}$$

For concentration polarization:

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

Pilling-Bedworth Ratio

For divalent metals:

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

For other than divalent metals:

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

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

(Metals) Conductivity for *n*-

 $\underline{\text{Type Extrinsic Semiconductor}}$

$$\sigma = n \ e \ \mu_e$$

(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

$$\sigma = n \ e \ \mu_e + p \ e \ \mu_h$$
$$= n_i \ e \ (\mu_e + \mu_h)$$

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

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

Materials

Dielectric Displacement

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

In a vacuum:

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

In a dielectric material:

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

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

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

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:

$$M_{\rm s} = 0.60 \mu_{\rm B} N$$

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

$$c = \lambda v$$

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

<u>Radiation</u>

$$I_T' = I_0' e^{-\beta x}$$

 \rightarrow Reflection losses not taken into account)

Intensity of Radiation

<u>Transmitted</u>

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

 \rightarrow Reflection losses taken into account)

Many equations were referenced from Callister, W. D. (2012). Materials science and engineering: An introduction 9E. John Wiley & Sons.