Advanced Materials formula booklet

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Atomic bonding (Lecture 1)

Fraction of ionic bonding	$$f_{ion} = 1 - e^{-\frac{(X_A - X_B)^2}{4}}$$ where X_A and X_B are the electronegativities of the two bonded elements

Crystallography and structure of metals (Lecture 2)

Atomic packing factor	$$APF = \frac{\text{volume of atoms in a unit cell}}{\text{total unit cell volume}}$$ Note that face atoms are counted as half atoms, and corner atoms are counted as eighth atoms
Unit cell edge length for body-centered cubic	$$a = \frac{4R}{\sqrt{3}}$$
Unit cell edge length for face-centered cubic	$$a = 2R\sqrt{2}$$
Density of a metal with a unit cell	$$\rho \approx \frac{\text{mass of atoms in a unit cell}}{\text{total unit cell volume}} = \frac{nA}{V_C N_A}$$ n is the number of atoms associated with each unit cell A is the atomic weight V_C is the volume of the unit cell N_A is Avogadro's number, $6.02 \cdot 10^{23}$ mol^{-1}
Density of a metal in terms of atomic packing factor	$$\rho \approx APF \cdot \rho_{atom} = APF \cdot \frac{m_{atom}}{V_{atom}}$$ where m_{atom} is the mass of a single atom and V_{atom} is the volume of a single atom
Atomic packing factors for cubic lattices	sc: $APF = 0.52$ bcc: $APF = 0.68$ fcc: $APF = 0.74$

Lattice defects (Lecture 3)

Equilibrium density of vacancies	$$c_V = \frac{N_V}{N} = e^{-\left(\frac{Q_V}{kT}\right)}$$ where N_V is the number of vacancies, N is the number of atomic sites, Q_V is the vacancy formation energy, and k is the Boltzmann constant, $1.38 \cdot 10^{-23}\ \mathrm{J/K}$
Number of atoms per unit volume	$$N = \frac{N_A \rho}{M}$$ where N_A is Avogadro's number, $6.02 \cdot 10^{23}\ \mathrm{mol^{-1}}$, ρ is density, and M is molar mass
Dislocation density	$$\rho = \frac{L}{V}$$ where L is dislocation line length and V is volume
Mass fraction/weight percentage for a binary alloy	$$C_A = \frac{m_A}{m_A + m_B}$$
Amount fraction/atomic percentage for a binary alloy	$$C_A^* = \frac{n_A}{n_A + n_B}$$ where n is number of moles
Conversion between mass fraction and amount fraction	$$C_A = \frac{C_A^* M_A}{C_A^* M_A + C_B^* M_B}$$ $$C_A^* = \frac{\frac{C_A}{M_A}}{\frac{C_A}{M_A} + \frac{C_B}{M_B}}$$ where M is molar mass

Ceramics and polymers (Lecture 4)

Determination of ceramic structure	$\frac{r_{A+}}{r_{X-}} < 0.414$: Zinc blende structure $0.414 < \frac{r_{A+}}{r_{X-}} < 0.732$: Sodium chloride structure $\frac{r_{A+}}{r_{X-}} > 0.732$: Cesium chloride structure r_{A+} is the radius of the cation and r_{X-} is the radius of the anion

Molar mass of polymer chain molecule	$$M = nM_{unit}$$ where n is the number of repeating units and M_{unit} is the molar mass of a single repeating unit
Number-weighted average molar mass	$$\langle M \rangle_n = \sum x_i M_i$$ where x_i is the fraction of all chains having molar mass M_i
Degree of polymerization (number of monomers in a chain)	$$DP = \frac{M}{M_{mon}}$$ where M is the molar mass of the chain and M_{mon} is the molar mass of a monomer For co-polymers: $$DP = \frac{M}{\langle M_{mon} \rangle}$$ where $\langle M_{mon} \rangle$ is the average molar mass of the monomers For a distribution of chain lengths: $$\langle DP \rangle = \frac{\langle M \rangle_n}{M_{mon}} \text{ or } \langle DP \rangle = \frac{\langle M \rangle_n}{\langle M_{mon} \rangle}$$ where the angle brackets denote an average. $\langle M \rangle_n$ is the *number-weighted* average molar mass
Straightened chain length	$$L = Nd \sin\left(\frac{\theta}{2}\right)$$ where N is the number of single bonds along the chain, d is the bond length, and θ is the bond angle
Average start to end distance for a polymer chain	$$r = d\sqrt{N}$$ where d is the bond length and N is the number of single bonds along the chain
Density of a semicrystalline polymer	$$\rho_{sc} = f_c \rho_c + (1 - f_c)\rho_a$$ where ρ_c is the density of the crystalline region, ρ_a is the density of the amorphous region, and f_c is the volume fraction of crystalline regions. Transposing for f_c, $$f_c = \frac{\rho_{sc} - \rho_a}{\rho_c - \rho_a}$$
Crystallinity	$$x = \frac{m_c}{m_{sc}} = \frac{f_c \rho_c}{\rho_{sc}} = \frac{\rho_c(\rho_{sc} - \rho_a)}{\rho_{sc}(\rho_c - \rho_a)}$$ where c is the crystalline region, a is the amorphous region, and sc is the whole semicrystalline polymer

Imaging (Lecture 5)

Interplanar spacing for a cubic crystal	$$d_{hkl} = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$$ where a is the unit cell edge length and h, k, and l are the Miller indices of the plane being considered
Bragg's law	$$n\lambda = 2d_{hkl}\sin(\theta)$$ n is the order of reflection, a positive integer λ is the x-ray wavelength 2θ, not θ, is the diffraction angle
Lens equation	$$\frac{1}{d_i} + \frac{1}{d_0} = \frac{1}{f}$$ where d_i is the distance from the lens to the image plane, d_0 is the distance from the lens to the object plane, and f is the focal length
Lens magnification	$$M = \frac{d_i}{d_0}$$
Mean intercept length for grain size	Draw many random lines. The mean intercept length is $$\bar{l} = \frac{L_T}{PM}$$ where L_T is the total length of all the lines, P is the total number of intercepts, and M is the magnification

Mechanical testing (Lecture 6)

Tensile/compressive stress	$$\sigma = \frac{F_t}{A_0}$$ where F_t is the force applied and A_0 is the initial cross sectional area of the specimen. $\sigma > 0$ for tensile stress and $\sigma < 0$ for compressive stress
Tensile/compressive strain	$$\varepsilon = \frac{\Delta l}{l_0}$$ where Δl is the elongation and l_0 is the initial specimen length
Hooke's law	$$\sigma = E\varepsilon$$ where E is the elastic modulus, or Young's modulus
Poisson's ratio	$$\nu = -\frac{\Delta d/d_0}{\Delta l/l_0} = -\frac{\varepsilon_x}{\varepsilon_z}$$ where d is the length perpendicular to a load and l is the length parallel to it

Shear stress	$$\tau = \frac{F_s}{A_0}$$
Shear strain	$$\gamma = \frac{\Delta x}{h_0}$$ where Δx is the displacement of one side and h_0 is the initial height
Hooke's law for shear	$$\tau = G\gamma$$ where G is the shear modulus
Relationship between moduli for elastic isotropic materials	$$G = \frac{E}{2(1+\nu)}$$

Electrical and thermal properties (Lecture 7)

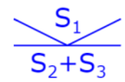
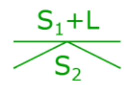
Resistance (Ohm's law)	$$R = \frac{V}{I}$$ Unit: Ω. V is voltage and I is current
Resistivity	$$\rho = \frac{RA}{L}$$ Unit: Ωm. A is cross-sectional area and L is length
Conductance	$$C = \frac{1}{R}$$ Unit: Ω^{-1}
Conductivity	$$\sigma = \frac{1}{\rho}$$ Unit: $(\Omega m)^{-1}$
Current density	$$J = \frac{I}{A}$$ Unit: A/m^2. A is cross-sectional area
Electric field intensity	$$\mathcal{E} = \frac{V}{L}$$ Unit: V/m. L is length
Current density in terms of electron density	$$J = n\lvert e\rvert v_d$$ where n is the electron density, $\lvert e\rvert$ is the absolute value of electron charge, $1.6 \cdot 10^{-19}$ C, and v_d is the net drift velocity
Net drift velocity	$$v_d = \mu_e \mathcal{E}$$ where μ_e is the electron mobility

Contributions to resistivity are additive	Total resistivity is the sum of resistivities due to temperature, impurities, and dislocations $$\rho_{total} = \rho_{temp} + \rho_{imp} + \rho_{disloc}$$
Intrinsic conductivity	$$\sigma = n_i\lvert e\rvert(\mu_e + \mu_h)$$ where n_i is the intrinsic carrier concentration, equal to both the electron concentration n and the hole concentration p. μ_e is electron mobility and μ_h is hole mobility
Extrinsic conductivity	For n-type: $$\sigma = n\lvert e\rvert\mu_e$$ For p-type: $$\sigma = p\lvert e\rvert\mu_h$$ n is electron concentration, p is hole concentration, μ_e and μ_h are electron and hole mobilities respectively, and $\lvert e\rvert$ is the absolute value of electron charge, $1.6 \cdot 10^{-19}\ \mathrm{C}$
Heat required for a temperature change	$$Q = mc\Delta T$$ $$Q = nC\Delta T$$ where c is specific heat capacity (per mass) and C is molar heat capacity. Heat capacities can be fixed-volume (c_v or C_v) or fixed-pressure (c_p or C_p)
Dependence of fixed-volume molar heat capacity on temperature at low temperatures	$$C_v = AT^3$$ where A is a constant For solid metallic elements, above the Debye temperature θ_D, C_v levels off at approximately $3R$, where R is the gas constant, $8.314\ \mathrm{J/(mol\ K)}$
Thermal expansion	Linear: $$\frac{\Delta L}{L_0} = \alpha_l \Delta T$$ where ΔL is the increase in length, L_0 is the initial length, and α_l is the linear expansion coefficient Volume: $$\frac{\Delta V}{V_0} = \alpha_v \Delta T$$ where ΔV is the increase in volume, V_0 is the initial volume, and α_v is the volume expansion coefficient
Thermal stress	$$\sigma = E\alpha_l \Delta T$$ where α_l is the linear expansion coefficient and E is the elastic modulus

Thermal shock resistance	$$TSR \approx \frac{\sigma_f k}{E\alpha_l}$$ where σ_f is fracture strength, k is thermal conductivity, E is the elastic modulus, and α_l is the linear expansion coefficient
Heat flux in steady state heat flow	$$q = \frac{\frac{dQ}{dt}}{A} = \frac{H}{A} = \frac{k(T_H - T_C)}{L}$$ H is heat current (power) A is the area through which the heat flows k is thermal conductivity T_H is the temperature of the hot end T_C is the temperature of the cold end L is the length of the heat flow path
Contributions to thermal conductivity are additive	Total conductivity is the sum of conductivities due to the lattice and due to free electrons $$k = k_{lattice} + k_{electron}$$
Relationship between electrical and thermal conductivity for metals (Wiedemann-Franz law)	$$L = \frac{k}{\sigma T}$$ where L is a constant which is approximately the same for all metals. k is thermal conductivity and σ is electrical conductivity. The theoretical value of L is $2.44 \cdot 10^{-8}\ \Omega\mathrm{W/K^2}$

Phase diagrams (Lecture 9)

Mass fraction of each phase in a two-phase region	$$W_A = \frac{\text{length from the point to the }\textbf{other}\text{ phase on the tie line}}{\text{total length of the tie line}} = \frac{\lvert c_B - c_0 \rvert}{\lvert c_B - c_A \rvert}$$
Gibbs phase rule	$$\text{number of degrees of freedom} + \text{number of phases in equilibrium} = \text{number of constituents} + 1$$

Special phase transformations	eutectic L → S_1 + S_2  eutectoid S_1 → S_2 + S_3  peritectic S_1 + L → S_2 

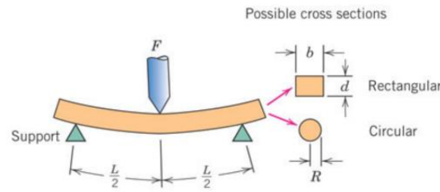
Plastic deformation and strengthening (Lecture 10)

Theoretical yield strength for a defect-free material	$$\sigma_{th} = \frac{E}{20}$$
Theoretical critical shear stress	$$\tau_{th} = \frac{G}{20}$$
Percent cold work	$$\%CW = \frac{A_0 - A_d}{A_0} \cdot 100\%$$ where A_0 is the original area of the cross-section that experiences deformation and A_d is the cross-sectional area after deformation
Total strength due to different factors is additive	$$\sigma = \sigma_0 + \Delta\sigma_{ss} + \Delta\sigma_{disl} + \Delta\sigma_{gb} + \Delta\sigma_p$$
Dependence of yield strength on work hardening	$$\sigma_y = \sigma_0 + \Delta\sigma_{disl} = \sigma_0 + M\alpha Gb\sqrt{\rho}$$ where M is the Taylor factor, α is the interaction coefficient, G is the shear modulus, and b is the length of the Burgers vector
Dependence of yield strength on grain size (Hall-Petch relation)	$$\sigma_y = \sigma + \Delta\sigma_{gb} = \sigma_0 + \frac{k_y}{\sqrt{d}}$$ where d is the average grain diameter and σ_0 and k_y are constants for a particular material

Contribution to yield strength from particle strengthening	Coherent: $$\Delta\sigma_{\mathrm{p,\,coh}} \propto \frac{\gamma r}{I + 2r}$$ where γ is the interface energy, I is the distance between particles, and r is the particle radius Incoherent: $$\Delta\sigma_{\mathrm{p,\,inchoh}} \propto \frac{Gb}{I}$$ where G is the shear modulus, b is the length of the Burgers vector, and I is the distance between particles
Relation between Brinell and Vickers hardness	$$HB \approx 0.95HV$$
Relation between ultimate tensile strength and Brinell hardness	$$UTS \approx c_{emp}HB$$ where c_{emp} is a constant that depends on material type

Failure (Lecture 11)

Maximum stress at a crack tip	$$\sigma_{max} \approx 2\sigma_0\sqrt{\frac{a}{\rho_t}}$$ where σ_0 is the applied stress, ρ_t is the radius of curvature of the crack tip, and a is either the length of a surface crack or half the length of an internal crack
Critical stress for crack propagation in a brittle material	$$\sigma_c = \sqrt{\frac{2E\gamma_s}{\pi a}}$$ where E is the elastic modulus, γ_s is the specific surface energy, and a is either the length of a surface crack or half the length of an internal crack
Fracture toughness	$$K_{Ic} = Y\sigma_c\sqrt{\pi a}$$ where Y is a parameter approximately equal to 1 for thick specimens, σ_c is the critical stress above, and a is either the length of a surface crack or half the length of an internal crack
Stress intensity factor	$$K_I = Y\sigma\sqrt{\pi a}$$ as for fracture toughness, but for any stress. Catastrophic crack growth occurs when $K_I \geq K_{Ic}$

Flexural strength	Rectangular cross-section: $$\sigma_{fs} = \frac{3F_f L}{2bd^2}$$ where F_f is the load at fracture, L is the distance between support points, and b and d are as indicated in the figure  Circular cross-section: $$\sigma_{fs} = \frac{F_f L}{\pi R^3}$$ where R is the radius of the specimen

Composites and material indices (Lecture 13)

Longitudinal elastic modulus for a fiber/lamellar composite or upper bound for all composites	$$E_{c\parallel} = f_1 E_1 + f_2 E_2$$ where f is volume fraction, E is elastic modulus, and the subscripts represent different phases. This situation is iso-strain
Ratio of load carried by fibers and the matrix phase for longitudinal loading	$$\frac{F_f}{F_m} = \frac{E_f f_f}{E_m f_m}$$ where f is volume fraction, E is elastic modulus, and the subscripts represent different phases
Transverse elastic modulus for a fiber/lamellar composite or lower bound for all composites	$$\frac{1}{E_{c\perp}} = \frac{f_1}{E_1} + \frac{f_2}{E_2}$$ where f is volume fraction, E is elastic modulus, and the subscripts represent different phases. This situation is iso-stress
Density of a composite	$$\rho_c = f_1 \rho_1 + f_2 \rho_2$$ where f is volume fraction and the subscripts represent different phases
General tensile stress for a fiber composite with longitudinal applied stress	$$\sigma(\varepsilon) = f_m \sigma_m(\varepsilon) + f_f \sigma_f(\varepsilon) = f_m \sigma_m(\varepsilon) + f_f E_f \varepsilon$$ where f is volume fraction, ε is strain, $\sigma(\varepsilon)$ is the stress of a phase at a certain strain, and E is elastic modulus. The subscript m represents the matrix and the subscript f represents the fibers

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<td>Yield strength of a fiber composite with longitudinal applied stress</td>
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$$\sigma_{\mathrm{y,\,c}} = f_m \sigma_{\mathrm{y,\,m}} + f_f E_f \varepsilon_{\mathrm{y,\,m}}$$

f_m and f_f are the volume fractions of the matrix and fibers respectively

$\sigma_{\mathrm{y,\,m}}$ is the yield strength of the matrix

E_f is the elastic modulus of the fibers

$\varepsilon_{\mathrm{y,\,m}}$ is the yield strain of the matrix

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<td>Tensile strength of a fiber composite with longitudinal applied stress</td>
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$$\sigma^* = f_m \sigma'_m + f_f \sigma^*_f$$

f_m and f_f are the volume fractions of the matrix and fibers respectively

σ'_m is the stress on the matrix at the failure strain of the fibers

σ^*_f is the fracture strength of the fibers

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<td>Material indices for lightweight structures</td>
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<tr><th>Member</th><th></th><th>Loading</th><th>Index</th></tr>
<tr><td>Beam</td><td>Stiffness</td><td>Tension / compression</td><td>E/ρ</td></tr>
<tr><td></td><td></td><td>Torsion</td><td>G/ρ</td></tr>
<tr><td></td><td></td><td>Bending</td><td>$E^{1/3}/\rho$ $E^{1/2}/\rho$</td></tr>
<tr><td></td><td>Buckling</td><td>Compression</td><td>$E^{1/2}/\rho$</td></tr>
<tr><td>Panel</td><td>Stiffness</td><td>Bending</td><td>$E^{1/3}/\rho$</td></tr>
<tr><td></td><td></td><td></td><td></td></tr>
<tr><td>Beam</td><td>Strength*</td><td>Tension / compression</td><td>σ_y/ρ</td></tr>
<tr><td></td><td>Strength*</td><td>Bending</td><td>$\sigma_y^{2/3}/\rho$</td></tr>
<tr><td>Panel</td><td>Strength*</td><td>Bending</td><td>$\sigma_y^{1/2}/\rho$</td></tr>
<tr><td>Spring</td><td>Resilience</td><td></td><td>$\sigma_y^2/E\rho$</td></tr>
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* Either yield strength or failure strength

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