Exam 1 Equations

Ch. 2 - Interatomic Forces

$$E_N = E_A + E_R = -\frac{A}{r} + \frac{B}{r^n}$$
 (1.1)

$$A = \frac{1}{4\pi\epsilon_0} \left(Z_1 e \right) \left(Z_2 e \right) \tag{1.2}$$

- \bullet This equation works for both A and B
- $\epsilon_0 = 8.85 \times 10^{-12} \text{F/m}$
- $e = 1.602 \times 10^{-19} \text{C}$
- \bullet r Radius in m

$$F_A = \frac{\left(1.602 \times 10^{-19}\right)^2}{4\pi \left(8.85 \times 10^{-12}\right) r^2} (\|Z_1\|) (\|Z_2\|) \tag{1.3}$$

- F_A Force of Attraction
- \bullet r Distance in m
- Z Number of Valence Electrons
- F_A Interatomic Force in N
- $-F_A = F_R$ Attractive and Repulsive Force Equal and Opposite

Force =
$$\frac{dE}{dr}$$
 (1.4)

Elastic Modulus =
$$\frac{dF}{dr}$$
 (1.5)

$$\%IC = \left(1 - e^{\frac{(x_A - x_B)^2}{4}}\right) \times 100\%$$
 (1.6)

- $\bullet~\% IC$ % Ionic Character
- \bullet x Electronegativities

Ch. 3 - Structures of Metals/Ceramics

1.2.1 Lattice Parameters

$$a_{\rm BCC} = \frac{4r}{\sqrt{3}} \tag{1.7}$$

$$a_{\text{FCC}} = \frac{4r}{\sqrt{2}} \tag{1.8}$$

$$a_{\rm HCP} = \frac{c}{1.633}$$
 (1.9)

- a Lattice Parameter
- r Radius of atom

Volume of Hexagonal Prism 1.2.2

$$V_H = \frac{3\sqrt{3}}{2}a^2h (1.10)$$

1.2.3 Densities

$$\rho = \frac{nA}{V_C N_A} \tag{1.11}$$

- n Number of atoms/unit cell
- A Molar Mass of Material
- $\bullet~V_C$ Volume of Unit Cell in cm

• N_A - Avogadro's Number (6.022×10^{23})

$$Planar Density = \frac{\frac{Atoms}{2D Unit Area}}{\frac{Area}{2D Repeat Unit}}$$
(1.12)

$$Linear Density = \frac{\# \text{ of Atoms in a Direction}}{Magnitude \text{ of Linear Vector}}$$
 (1.13)

• The repeat units/vector magnitude are in terms of atomic

$$APF = \frac{\frac{Atoms}{Unit \text{ Cell}} \left(\frac{4}{3}\pi \left(atom \text{ radius}\right)^{3}\right)}{Unit \text{ Cell Volume}}$$
(1.14)

Thermal Expansion

$$\frac{\Delta L}{L_0} = \alpha \left(T_2 - T_1 \right) \tag{1.15}$$

- $E \uparrow$, $T_m \uparrow$
- $E \uparrow$, $\alpha \downarrow$

Convert between Coordinates

$$a_{1} = \frac{1}{3}(2X - Y)$$

$$a_{2} = \frac{1}{3}(2Y - X)$$

$$a_{3} = -(a_{1} + a_{2})$$

$$c = Z$$

$$a_{1} + a_{2} + a_{3} = 0$$

$$(1.16)$$

1.2.6 Planes

- 1. Given x, y, z as intersects
- 2. Convert to $\frac{1}{x}$, $\frac{1}{y}$, $\frac{1}{z}$ 3. Reduce to smallest common denominator 4. Leave as $\left(\frac{1}{x}, \frac{1}{y}, \frac{1}{z}\right)$

1.2.7 Light Refraction

$$D = \frac{n\lambda}{2\sin\theta} \tag{1.17}$$

- n = 1
- λ Wavelength in nm
- θ Angle of Incidence
- θ is usually given as 2θ . Be careful

1.2.8 Randoms

$$D_{HKL} = \frac{a}{\sqrt{h^2 + k^2 + l^2}} \tag{1.18}$$

• ONLY for cubic structures

2 Exam 2 Equations

2.1 Ch. 4 Imperfections

2.1.1 Vacancies

Number of Vacancies:

$$N_V = ext{Vacancy Frac.} imes rac{N_A
ho_{ ext{Ele}}}{A_{ ext{Ele}}}$$

- A_{Ele} Atomic Weight (g/mol)
- $\rho_{\rm Ele}$ Element Density (g/c³m)
- N_A Avogadro's Number (6.022×10^{23})

Number of Potential Vacancy Sites:

$$N = \frac{\rho_{\rm Ele} N_A}{A_{\rm Ele}}$$

- $A_{\rm Ele}$ Atomic Weight (g/mol)
- $\rho_{\rm Ele}$ Element Density (g/c³m)
- N_A Avogadro's Number (6.022×10^{23})

Grains per Area:

$$n_M = \left(\frac{100}{M}\right)^2 = 2^{G-1}$$

- n_M Grains/in²
- \bullet G Grain Size Number

$$-G = -6.6457 \log (\bar{\ell}) - 3.298$$
 for mm $-G = -6.6353 \log (\bar{\ell}) - 12.6$ for in.

2.1.2 Mean Intercept Length

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

- L_T Total Length of all Lines
- $\bullet~P$ Number of Grain Intersections
- ullet M Magnification

$$M = \frac{\text{Scale Length}}{\# \text{ on Scale Bar}}$$
 (2.5)

2.1.3 Complete Substitution

To have a complete substitution, it must be:

- $\Delta r < 15\%$
- Electronegativity $\leq .4$
- SAME Crystal Structure
- SAME Valence

2.1.4 Edges

Burger's Vector:

- Burger's Vector
 - \perp for Edge Dislocations
 - − || for Screw Dislocations
- Twin Boundary Symmetric Around Fault
- Stacking Fault NOT Symmetric Around Fault
 - High Angle $E \uparrow$
 - Low Angle $E \downarrow$

2.2 Ch. 5 Diffusion

2.2.1 Diffusion Coefficient

$$D = D_0 \times e^{\frac{-Q_d}{RT}} \tag{2.6}$$

- D Diffusion Coefficient (m²/s)
- Q_d Activation Energy (J/mol, eV/atom)
- (2.1) R 8.314 (J/molK)
 - T Temperature (K)

$$D_1 t_1 = D_2 t_2 (2.7)$$

- \bullet D Diffusion Coefficients
- \bullet t Time

(2.2) **2.2.2** Flux

(2.3)

$$J = -DA\frac{dC}{dx} \tag{2.8}$$

- For Steady State Diffusion
- ullet D Diffusion Coefficient
- dC Δ Concentration (Low-High)
- \bullet dx Distance to Cross
- \bullet A Area

2.2.3 Diffusion Concentration

$$\frac{C(x,t) - C_0}{C_s - C_0} = 1 - \operatorname{erf}\left(\frac{x}{2\sqrt{Dt}}\right)$$
 (2.9)

$$Z = \frac{x}{2\sqrt{Dt}} = \frac{z - \text{point below}}{\text{point above - point below}}$$
 (2.10)

- C(x,t) Concentration at a point AND time
- C_0 Initial Concentration
- (2.4) C_2 Surface Concentration of DIFFUSING species
 - \bullet x Position
 - ullet D Diffusion Coefficient
 - \bullet t Time

3 Exam 3 Equations

3.1 Ch. 6 - Mechanical Properties

3.1.1 Stress

Tensile Stress

$$\sigma = \frac{F_t}{A_0} \tag{3.1}$$

- Think of amount of force required to pull ends of paper apart
- σ has units lb_f/in^2 or N/m²
- F_t Normal Force
- A_0 Original Cross-Sectional Area
- $\sigma < 0$ Compressive Force
- $\sigma > 0$ Tensile Force

Shear Stress

$$\tau = \frac{F_S}{A_0} \tag{3.2}$$

- Think of amount of force required to rip a piece of paper
- τ has units lb_f/in^2 or N/m²
- F_S Shear Force
- A_0 Original Cross-Sectional Area

3.1.2 Strain

Tensile Strain

$$\varepsilon = \frac{\delta}{L_0} = \frac{L - L_0}{L_0} \tag{3.3}$$

- Think of pulling ends of paper apart and seeing how much it stretches
- ε Tensile Strain
- δ Change in Length of Material
- L_0 Original Length of Material

Shear Strain

$$\gamma = \frac{\Delta x}{y} = \tan \theta \tag{3.4}$$

- Change of length of material compared to height when ripped apart
- γ Shear Strain
- Δx Change in length
- y Height of Material Tested

3.1.3 Moduli

Young's Modulus

$$E = \frac{\sigma}{\varepsilon} = \frac{dF}{dr} \tag{3.5}$$

- How Stiff a Material is from being pulled apart
- E Young's Modulus
- \bullet σ Tensile Stress
- ε Tensile Strain

Elastic Shear Modulus

$$G = \frac{\tau}{\gamma} \tag{3.6}$$

- How Stiff a material is from Ripping
- τ Shear Stress
- γ Shear Strain

Elastic Bulk Modulus

$$K = -P\frac{V_0}{\Delta V} \tag{3.7}$$

- ullet K Elastic Bulk Modulus
- P -
- V_0 Original Volume

Poisson's Ratio

$$v = -\frac{\varepsilon_L}{\varepsilon} \tag{3.8}$$

- ullet v Poisson's Ratio
- ε_L Tensile Strain at the length L
- ε Tensile Strain

3.1.4 Isotropic Materials

If a material is isotropic, these equations apply to Elastic Shear Modulus and Elastic Bulk Modulus.

$$G = \frac{E}{2(1+v)} \tag{3.9}$$

$$K = \frac{E}{3(1 - 2v)} \tag{3.10}$$

- ullet G Elastic Shear Modulus of isotropic material
- $\bullet~K$ Elastic Bulk Modulus of isotropic material
- \bullet E Young's Modulus of material
- ullet v Poisson's Ratio of Material

3.1.5 Deflection

$$\delta = \frac{FL_0}{EA_0} \tag{3.11}$$

- F Force Applied
- L_0 Original Length of Material
- ullet E Young's Modulus
- \bullet A_0 Original Cross-Sectional Area of Material

Simple Tension

$$\delta_L = -v \frac{Fw_0}{EA_0} \tag{3.12}$$

- $delta_L$??
- ullet v Poisson's Ratio
- \bullet F Force Applied
- w_0 Width of Thing applying the force
- \bullet E Young's Modulus
- ullet A_0 Original Cross-Sectional Area of Material

3.1.6 Simple Torsion

$$\alpha = \frac{2ML_0}{\pi (r_0)^4 G}$$
 (3.13)

- α Simple Torsion
- M -
- L_0 Original Length of Material
- \bullet r_0 -
- ullet G Elastic Shear Modulus

3.1.7 Working with Stress Curve

- $\sigma_u = \text{Yield Strength}$
- Tensile Strength = Max Height on Curve (Plastic Defor-
- Toughness = Area Beneath the Stress Curve (Energy Absorbed)
- Percent Elongation (%EL)
- Percent Reduction in Area
- $U_r \cong \frac{1}{2}\sigma_y \varepsilon_y = \text{Resilience}$ (Energy Absorbed in Elastic
- $\sigma_T = \frac{F}{A_0} = K \varepsilon_T^n = \text{True Stress}$
- $\epsilon_T = \ln\left(\frac{L}{L_0}\right) = \text{True Strain}$ $\sigma_{\text{Working}} = \frac{\sigma_y}{N} = \text{Safety Measure Measure}$

Percent Elongation (%EL)

$$\%EL = \frac{L_f - L_0}{L_0} \times 100\% \tag{3.14}$$

- %EL Percent Elongation
- \bullet L_f Final Length of Material
- L_0 Starting Length of Material

Percent Reduction in Area

$$\%RA = \frac{A_0 - A_f}{A_0} \times 100\% \tag{3.15}$$

- %RA Percent Reduction in Area
- A_f Final Cross-Sectional Area of Material
- A_0 Starting Cross-Sectional Area of Material

Random Equations 3.1.8

$$HB = \frac{2P}{\pi D \left(D - \sqrt{D^2 - d^2}\right)} \tag{3.16}$$

$$HV = 1.854 \times \frac{P}{d^2} \tag{3.17}$$

$$HK = 14.2 \times \frac{P}{I^2}$$
 (3.18)

Ch. 7 - Deformation & Strengthening Mechanisms

Burger's Vector Explained

$$\|\vec{b}\| = \frac{a}{2}\sqrt{u^2 + v^2 + w^2}$$

$$\vec{b}_{BCC} = \frac{a}{2} [111]$$

$$\vec{b}_{FCC} = \frac{a}{2} [110]$$

$$\vec{b}_{HCP} = \frac{a}{2} [11\bar{2}0]$$
(3.19)

3.2.2 Angled Stresses

$$\phi/\lambda = \arccos\left(\frac{u_1u_2 + v_1v_2 + w_1w_2}{\sqrt{(u_1^2 + v_1^2 + w_1^2)(u_2^2 + v_2^2 + w_2^2)}}\right) \quad (3.20)$$

- ϕ Angle of stress to normal
- λ Angle of stress to slip direction

3.2.3 Strengthening Mechanisms

- 1. Grain-Size Reduction Increase grain boundaries, increase misalignment
- 2. Solid-Solution Add interstitial atoms
- 3. Cold Work/Annealing Increase the number of disloca-
- 4. Precipitation Strengthening Shear precipitate or bend the slip line

Grain-Size Reduction

$$\sigma_y = \sigma_0 + k dy^{\frac{-1}{2}} \tag{3.21}$$

- $\begin{array}{l} \bullet \;\; \rho_{\rm disloc} \uparrow = \sigma_y \uparrow \\ \bullet \;\; \rho_{\rm disloc} = \frac{{\rm Total \; disloc. \; Length}}{{\rm Unit \; Volume}} \\ \end{array}$

Solid-Solution

$$\sigma_y = c^{\frac{1}{2}} \tag{3.22}$$

• c - Impurity Concentration

Cold Work/Annealing

$$\%CW = \frac{A_0 - A}{A_0} \times 100 \tag{3.23}$$

$$d^n - d_0^n = kt (3.24)$$

- Equation (3.24) only works if heat treatment occurs
- n=2, usually

Precipitation Strengthening

$$\sigma_y = \frac{1}{s} \tag{3.25}$$

• s - Space in pinning sites

- 4 Exam 4 Equations
- 4.1 Ch. 9 Phase Diagrams
- 4.2 Ch. 10 Phase Transformations

- 5 Exam 5 Equations
- 5.1 Ch. 12/15 Mechanical Properties of Ceramics and Polymers
- 5.2 Ch. 18 Electrical Properties

A Trigonometry

A.1 Trigonometric Formulas

$$\sin\left(\alpha\right) + \sin\left(\beta\right) = 2\sin\left(\frac{\alpha+\beta}{2}\right)\cos\left(\frac{\alpha-\beta}{2}\right) \qquad (A.1) \qquad \cos\left(\alpha\right) + \cos\left(\alpha\right) = 2\cos\left(\frac{\alpha+\beta}{2}\right)\cos\left(\frac{\alpha-\beta}{2}\right)$$

$$\cos(\theta)\sin(\theta) = \frac{1}{2}\sin(2\theta) \qquad (A.2) \qquad \cos(\alpha) - \cos(\beta) = -2\sin\left(\frac{\alpha+\beta}{2}\right)\sin\left(\frac{\alpha-\beta}{2}\right)$$

A.9 Pythagorean Theorem for Trig

Polar to Rectangular

Sum-to-Product Identities

 $\sin(\alpha) \pm \sin(\beta) = 2\sin\left(\frac{\alpha \pm \beta}{2}\right)\cos\left(\frac{\alpha \mp \beta}{2}\right)$

$$\cos^2(\alpha) + \sin^2(\alpha) = 1^2 \tag{A.23}$$

 $re^{i\theta} = r\cos(\theta) + ir\sin(\theta)$

A.2 Euler Equivalents of Trigonometric A.9 Functions

$$e^{\pm i\alpha} = \cos(\alpha) \pm i\sin(\alpha)$$
 (A.3)

$$\sin\left(x\right) = \frac{e^{ix} + e^{-ix}}{2} \tag{A.4}$$

$$\cos\left(x\right) = \frac{e^{ix} - e^{-ix}}{2i} \tag{A.5}$$

$$\sinh\left(x\right) = \frac{e^x - e^{-x}}{2} \tag{A.6}$$

$$\cosh\left(x\right) = \frac{e^x + e^{-x}}{2} \tag{A.7}$$

A.10 Rectangular to Polar

A.11

$$a + ib = \sqrt{a^2 + b^2}e^{i\theta} = re^{i\theta} \tag{A.24}$$

(A.20)

(A.21)

(A.22)

(A.26)

$$\theta = \begin{cases} \arctan\left(\frac{b}{a}\right) & a > 0\\ \pi - \arctan\left(\frac{b}{a}\right) & a < 0 \end{cases}$$
 (A.25)

A.3 Angle Sum and Difference Identities

$$\sin(\alpha \pm \beta) = \sin(\alpha)\cos(\beta) \pm \cos(\alpha)\sin(\beta) \tag{A.8}$$

$$\cos(\alpha \pm \beta) = \cos(\alpha)\cos(\beta) \mp \sin(\alpha)\sin(\beta) \tag{A.9}$$

A.4 Double-Angle Formulae

$$\sin(2\alpha) = 2\sin(\alpha)\cos(\alpha) \tag{A.10}$$

$$\cos(2\alpha) = \cos^2(\alpha) - \sin^2(\alpha) \tag{A.11}$$

A.5 Half-Angle Formulae

$$\sin\left(\frac{\alpha}{2}\right) = \sqrt{\frac{1 - \cos\left(\alpha\right)}{2}} \tag{A.12}$$

$$\cos\left(\frac{\alpha}{2}\right) = \sqrt{\frac{1 + \cos\left(\alpha\right)}{2}} \tag{A.13}$$

A.6 Exponent Reduction Formulae

$$\sin^2(\alpha) = \frac{1 - \cos(2\alpha)}{2} \tag{A.14}$$

$$\cos^2(\alpha) = \frac{1 + \cos(2\alpha)}{2} \tag{A.15}$$

A.7 Product-to-Sum Identities

$$2\cos(\alpha)\cos(\beta) = \cos(\alpha - \beta) + \cos(\alpha + \beta) \tag{A.16}$$

$$2\sin(\alpha)\sin(\beta) = \cos(\alpha - \beta) - \cos(\alpha + \beta) \tag{A.17}$$

$$2\sin(\alpha)\cos(\beta) = \sin(\alpha + \beta) + \sin(\alpha - \beta) \tag{A.18}$$

$$2\cos(\alpha)\sin(\beta) = \sin(\alpha + \beta) - \sin(\alpha - \beta) \tag{A.19}$$