1 Exam 1 Equations

$$E_N = E_A + E_R$$

$$F_A = \frac{\left(1.602 \times 10^{-19}\right)^2}{4\pi \left(8.85 \times 10^{-12}\right) r^2} \left(\|Z_1\|\right)\left(\|Z_2\|\right) \tag{1.1}$$

- r - Distance in m
- Z - Number of Valence Electrons
- F_A - Interatomic Force in N

$$\text{Force} = \frac{dE}{dr} \tag{1.2}$$

$$\text{Elastic Modulus} = \frac{dF}{dr} \tag{1.3}$$

1.1 Lattice Parameters

$$a_{\text{BCC}} = \frac{4r}{\sqrt{3}} \tag{1.4}$$

$$a_{\text{FCC}} = \frac{4r}{\sqrt{2}} \tag{1.5}$$

$$a_{\text{HCP}} = \frac{c}{1.633} \tag{1.6}$$

- a - Lattice Parameter
- r - Radius of atom

1.2 Volume of Hexagonal Prism

$$V_H = \frac{3\sqrt{3}}{2} a^2 h \tag{1.7}$$

1.3 Densities

$$\rho = \frac{nA}{V_C N_A} \tag{1.8}$$

- n - Number of atoms/unit cell
- A - Molar Mass of Material
- V_C - Volume of Unit Cell in cm
- N_A - Avogadro's Number (6.022×10^{23})

$$\text{Planar Density} = \frac{\frac{\text{Atoms}}{\text{2D Unit Area}}}{\frac{\text{Area}}{\text{2D Repeat Unit}}} \tag{1.9}$$

$$\text{Linear Density} = \frac{\text{\# of Atoms in a Direction}}{\text{Magnitude of Linear Vector}} \tag{1.10}$$

- The repeat units/vector magnitude are in terms of atomic radii

$$\text{APF} = \frac{\frac{\text{Atoms}}{\text{Unit Cell}} \left(\frac{4}{3}\pi \left(\text{atom radius}\right)^3\right)}{\text{Unit Cell Volume}} \tag{1.11}$$

$$\%\text{IC} = \left(1 - e^{\frac{(x_A - x_B)^2}{4}}\right) \times 100\% \tag{1.12}$$

- x - Electronegativities

1.4 Thermal Expansion

$$\frac{\Delta L}{L_0} = \alpha \left(T_2 - T_1\right) \tag{1.13}$$

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

1.5 Convert between Coordinates

$$[XYZ] = [a_1 a_2 a_3 c] \qquad \begin{aligned} a_1 &= \frac{1}{3}\left(2X - Y\right) \\ a_2 &= \frac{1}{3}\left(2Y - X\right) \\ a_3 &= -\left(a_1 + a_2\right) \\ c &= Z \end{aligned} \tag{1.14}$$

$$a_1 + a_2 + a_3 = 0$$

1.6 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 $\left(\frac{1}{x}\frac{1}{y}\frac{1}{z}\right)$

1.7 Light Refraction

$$D = \frac{n\lambda}{2\sin\theta} \tag{1.15}$$

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

1.8 Randoms

$$D_{HKL} = \frac{a}{\sqrt{h^2 + k^2 + l^2}} \tag{1.16}$$

- ONLY for cubic structures

2 Exam 2 Equations

2.1 Ch. 4 Imperfections

2.1.1 Vacancies

Number of Vacancies:

$$N_V = \text{Vacancy Frac.} \times \frac{N_A \rho_{\text{Ele}}}{A_{\text{Ele}}} \tag{2.1}$$

- A_{Ele} - Atomic Weight (g/mol)
- ρ_{Ele} - Element Density (g/c^{3}m)
- N_A - Avogadro's Number (6.022×10^{23})

Number of Potential Vacancy Sites:

$$N = \frac{\rho_{\text{Ele}} N_A}{A_{\text{Ele}}} \tag{2.2}$$

- A_{Ele} - Atomic Weight (g/mol)
- ρ_{Ele} - Element Density (g/c^{3}m)
- N_A - Avogadro's Number (6.022×10^{23})

Grains per Area:

$$n_M = \left(\frac{100}{M}\right)^2 = 2^{G-1} \tag{2.3}$$

- n_M - Grains/in^2
- G - Grain Size Number
  - $G = -6.6457 \log\left(\bar{\ell}\right) - 3.298$ for mm
  - $G = -6.6353 \log\left(\bar{\ell}\right) - 12.6$ for in.

2.1.2 Mean Intercept Length

$$\bar{\ell} = \frac{L_T}{PM} \tag{2.4}$$

- L_T - Total Length of all Lines
- P - Number of Grain Intersections
- M - Magnification

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

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 (m^2/s)
- Q_d - Activation Energy (J/mol, eV/atom)
- R - 8.314 (J/molK)
- T - Temperature (K)

$$D_1 t_1 = D_2 t_2 \tag{2.7}$$

- D - Diffusion Coefficients
- t - Time

2.2.2 Flux

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

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

2.2.3 Diffusion Concentration

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

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

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

A Trigonometry

A.1 Trigonometric Formulas

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

$$\cos(\theta)\sin(\theta) = \frac{1}{2}\sin(2\theta) \tag{A.2}$$

A.2 Euler Equivalents of Trigonometric Functions

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

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

$$\cos(x) = \frac{e^{\imath x} - e^{-\imath x}}{2\imath} \tag{A.5}$$

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

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

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

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

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

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

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

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

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

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

A.8 Sum-to-Product Identities

$$\sin(\alpha) \pm \sin(\beta) = 2\sin\left(\frac{\alpha\pm\beta}{2}\right)\cos\left(\frac{\alpha\mp\beta}{2}\right) \tag{A.20}$$

$$\cos(\alpha) + \cos(\alpha) = 2\cos\left(\frac{\alpha+\beta}{2}\right)\cos\left(\frac{\alpha-\beta}{2}\right) \tag{A.21}$$

$$\cos(\alpha) - \cos(\beta) = -2\sin\left(\frac{\alpha+\beta}{2}\right)\sin\left(\frac{\alpha-\beta}{2}\right) \tag{A.22}$$

A.9 Pythagorean Theorem for Trig

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

A.10 Rectangular to Polar

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

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

A.11 Polar to Rectangular

$$re^{\imath\theta} = r\cos(\theta) + \imath r\sin(\theta) \tag{A.26}$$