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

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

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

- 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

$$[XYZ] = [a_1 a_2 a_3 c] \qquad \begin{aligned} a_1 &= \frac{1}{3}\left(2X - Y\right) \\ a_2 &= \frac{1}{3}\left(2Y - X\right) \\ a_3 &= -\left(a_1 + a_2\right) \\ c &= Z \\ a_1 + a_2 + a_3 &= 0 \end{aligned} \tag{1.14}$$

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

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

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

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