1 Atomic Structure

1.1 Energy

$$u_v dv = \frac{8\pi v^2}{c^3} \cdot \frac{hv}{e^{\frac{hv}{K_b T}} - 1} \tag{1}$$

$$E = hv \tag{2}$$

1.2 Photoelectric Effect

$$\frac{1}{2} m_e v_k^2 = E_k = hv - W \tag{3}$$

$$\frac{1}{\lambda} = R_H \left(\frac{1}{n_1^2} - \frac{1}{n_2^2} \right) \tag{4}$$

$$R_H = 1.097373 \times 10^7 m^{-1} \tag{5}$$

$$n_1 = 1 \Rightarrow Lyman \tag{6}$$

$$n_1 = 2 \Rightarrow Balmer \tag{7}$$

$$n_1 = 3 \Rightarrow Paschen \tag{8}$$

$$n_1 = 4 \Rightarrow Brackett \tag{9}$$

$$n_1 = 5 \Rightarrow Pfund \tag{10}$$

$$n_2 > n_1 \tag{11}$$

1.3 De Broglie Relationship

$$E^2 = p^2 c^2 + m^2 c^4 \tag{12}$$

$$\text{for zero rest mass: } E^2 = p^2 c^2 \rightarrow E = pc \tag{13}$$

$$hv = h\frac{c}{\lambda} = pc \tag{14}$$

$$\therefore p = \frac{h}{\lambda} \tag{15}$$

1.4 Electron diffraction

$$E_K = eV - \frac{p^2}{2m} \tag{16}$$

$$p = \sqrt{2meV} \tag{17}$$

$$\lambda = \frac{h}{\sqrt{2meV}} \tag{18}$$

$$\lambda = 2d\sin(\theta) \tag{19}$$

$$\sin^2(\theta) = \frac{C}{V}, \text{ Where } C = \frac{h^2}{8med^2} \tag{20}$$

1.5 Bohr Model

$$F_{centripedal} = F_{electric} \tag{21}$$

$$m\frac{v^2}{r} = \frac{e^2}{4\pi\epsilon_0 r^2} \tag{22}$$

$$\therefore v^2 = \frac{e^2}{4\pi\epsilon_0 mr} \tag{23}$$

$$I_{orbit} = n\lambda = 2\pi r \text{ Where n is the quantisation condition} \tag{24}$$

$$\therefore v = \frac{hn}{2\pi mr} \tag{25}$$

$$L = mvr = n\frac{h}{2\pi} = n\hbar \tag{26}$$

As such, allowed radii are described by the expression: (27)

$$r_n = \frac{h^2\epsilon_0 n^2}{\pi me^2} = a_{Bohr}n^2 \tag{28}$$

$$r_1 = a_{Bohr} = \frac{h^2\epsilon_0}{\pi me^2} = 5.3 \times 10^{-11} m \tag{29}$$

$$E_k = \frac{1}{2}mv^2 = \frac{e^2}{8\pi\epsilon_0 r} \tag{30}$$

$$E_T = E_k + E_c = \frac{e^2}{8\pi\epsilon_0 r} - \frac{e^2}{4\pi\epsilon_0 r^2} = -\frac{e^2}{8\pi\epsilon_0 r} \tag{31}$$

Substiting in r_n gives: (32)

$$E_T = -\left(\frac{me^4}{8\epsilon_0^2 h^2}\right)\cdot\frac{1}{n^2} = \frac{-13.6eV}{n^2},\ 1\ eV \approx 1.602 \times 10^{-19} J \tag{33}$$

$$\Delta E = E_i - E_f = \frac{me^4}{8\epsilon_0^2 h^2}(\frac{1}{n_f^2} - \frac{1}{n_i^2}) \tag{34}$$

$$\text{since: } E = hv = h\frac{c}{\lambda} \tag{35}$$

$$\frac{1}{\lambda} = \frac{me^4}{8\epsilon_0^2 h^3}\left(\frac{1}{n_f^2} - \frac{1}{n_i^2}\right) = R_H\left(\frac{1}{n_f^2} - \frac{1}{n_i^2}\right) \tag{36}$$

1.6 Waves

$$\Psi = Ae^{i(kx-\omega t)} \tag{37}$$

$$k = 2\pi/\lambda \tag{38}$$

$$\omega = 2\pi v \tag{39}$$

$$c = v\lambda = \frac{\omega}{2\pi} \cdot \lambda = \frac{\omega}{\lambda} \tag{40}$$

$$P(x) \propto |\Psi|^2 dx \tag{41}$$

$$\frac{\partial \Psi}{\partial x} = ikAe^{i(kx-\omega t)} = ik\Psi \tag{42}$$

$$\frac{\partial \Psi}{\partial t} = -i\omega Ae^{i(kx-\omega t)} = i\omega\Psi \tag{43}$$

$$\text{De Broglie: } p = \frac{h}{\lambda} = \frac{h}{2\pi} \cdot \frac{2\pi}{\lambda} = \hbar k \tag{44}$$

$$\text{Enstein: } E = hv = h\frac{\omega}{2\pi} = \hbar\omega \tag{45}$$

$$\frac{\partial}{\partial x}\Psi = i\frac{p}{\hbar}\Psi \Rightarrow p\Psi = \{-i\hbar\frac{\partial}{\partial x}\}\Psi \tag{46}$$

$$\frac{\partial}{\partial t}\Psi = -i\frac{E}{\hbar}\Psi \Rightarrow E\Psi = \{i\hbar\frac{\partial}{\partial t}\}\Psi \tag{47}$$

$$\Delta t = \frac{1}{\Delta f} = \frac{h}{\Delta E} \Rightarrow \Delta E \cdot \Delta t \geq h \tag{48}$$

$$\Delta x = \Delta\lambda_{dB} = \frac{h}{\Delta p} \Rightarrow \Delta x \cdot \Delta p \geq h \tag{49}$$

Heisenber's Uncertainty Principle:

It is impossible to specify simultaneously, with precision, both the momentum and the position of a particle.

1.7 Shrodinger's Equation Derivation

$$E = E_k + E_p = \frac{1}{2}mv^2 + V = \frac{p^2}{2m} + V \tag{50}$$

$$i\hbar\frac{\partial}{\partial t}\Psi(x,t) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\Psi(x,t) + V\Psi(x,t) \tag{51}$$

1.8 Time independent Shrodinger's Equation

$$\Psi(x,t) = \phi(t)\psi(t) \tag{52}$$

$$i\hbar\frac{1}{\phi(t)}\frac{\partial\phi(t)}{\partial t} = -\frac{\hbar^2}{2m\psi(x)}\frac{\partial^2\psi(x)}{\partial x^2} + V \tag{53}$$

$$\therefore\ i\frac{A}{\hbar}\phi = \frac{\partial\phi(t)}{\partial t} \tag{54}$$

$$\phi(t) = Ce^{-i(\frac{A}{\hbar})t} \Rightarrow \frac{d\phi(t)}{dt} = -i(\frac{A}{\hbar})Ce^{-i(\frac{A}{\hbar})t} \tag{55}$$

$$\text{By unit analysis: } A = E \tag{56}$$

$$\therefore\ E\psi = -\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V\psi \tag{57}$$

1.9 Electron in a box

$$V(0) = V(L) = \inf \tag{58}$$

$$V(x) = 0\ \forall\, x\,|\,0 < x < L \tag{59}$$

$$\therefore\ -\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi \tag{60}$$

$$\text{General Solution: } \psi = A\sin(kx) + B\cos(kx) \tag{61}$$

$$\frac{d^2\psi}{dx^2} = -k^2(A\sin(kx)) + B\cos(kx)) = -k^2\psi \tag{62}$$

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = \left(-\frac{\hbar^2}{2m}\right)\cdot(-k^2\psi) = E\psi \tag{63}$$

$$E = \frac{\hbar^2k^2}{2m} \tag{64}$$

$$\text{Applying boundary conditions:} \tag{65}$$

$$\psi(0) = 0 \Rightarrow B = 0 \tag{66}$$

$$\psi(L) = 0 \Rightarrow A = 0\ or\ \sin(kL) = 0 \tag{67}$$

$$\therefore kL = n\pi,\ n = 1,2,3... \tag{68}$$

$$\psi_n = A\sin(\frac{n\pi x}{L}) \tag{69}$$

$$E_n = \frac{h^2}{8mL^2}\cdot n^2 \tag{70}$$

$$1 = \int_0^L A^2\sin^2(\frac{n\pi x}{L})dx \Rightarrow A = \sqrt{\frac{2}{L}} \tag{71}$$

$$\psi_n = \sqrt{\frac{2}{L}}\sin(\frac{n\pi x}{L}) \tag{72}$$

$$P_n(x) = \frac{2}{L}\sin^2(\frac{n\pi x}{L})dx \tag{73}$$

1.10 3D

$$-\frac{\hbar^2}{2m}\left(\frac{d^2}{dx^2}+\frac{d^2}{dy^2}+\frac{d^2}{dz^2}\right)\psi+V\psi=E\psi \tag{74}$$

$$\nabla=\left(\frac{d}{dx}+\frac{d}{dy}+\frac{d}{dz}\right) \tag{75}$$

$$-\frac{\hbar^2}{2m}\nabla^2\psi+V\psi=E\psi \tag{76}$$

There are 3 spacial degrees of freedom and 1 spin degree of freedom, therefore there are 4 quantum numbers

n = Principle quantum numbers, $\{n \,|\, n \in \mathbb{N}\}$

ℓ = Orbital quantum number $\{\ell \,|\, 0 \leq \ell \leq n-1,\ \ell \in \mathbb{W}\}$

m_ℓ = Magnetic quantum number $\{m_\ell \,|\, -\ell \leq m_\ell \leq \ell,\ m_\ell \in \mathbb{Z}\}$

m_s = Spin quantum number $\{m_s \,|\, m_s \in \{\frac{1}{2}, -\frac{1}{2}\}\}$

2 Bonding and Crystaline Structure

Bond	**Action with Charges**	**ΔE**	**E_{avg}**	**Bond Energy**
Ionic	Exchange	High	Low	Large
Covalent	Sharing	Low	High	Variable
Metalic	Delocalized Sharing	Low	Low	Variable

2.1 I don't have a good title yet

$$E_N = E_A + E_R = -\frac{A}{r}+\frac{B}{r^n} \tag{77}$$

$$ionic\ character = 1 - e^{-\frac{(X_A - X_B)^2}{4}} \tag{78}$$

$$\frac{\Delta L}{L_0} = \alpha\,(T_2 - T_1) \tag{79}$$

$$APF = \frac{n_a \cdot \frac{4}{3}\pi r_a^3}{a^3} \tag{80}$$

Structure	**Coordination Number**	**Atoms/unit cell**	**APF**
Simple Cubic	6	8	0.52
Body Centered Cubic (BCC)	8	2	0.68
Face Centered Cubic	12	4	0.74

2.2 Some densities

$$\rho = \frac{nA}{V_c N_a} \tag{81}$$

$$LD = \frac{n_a}{r} \tag{82}$$

$$PD = \frac{n}{a^2} \tag{83}$$

2.3 X-Ray Diffraction

$$d = \frac{n\lambda}{2\sin(\theta_c)} \tag{84}$$

$$d = \frac{a}{\sqrt{i^2 + j^2 + k^2}} \tag{85}$$

d = planar spacing

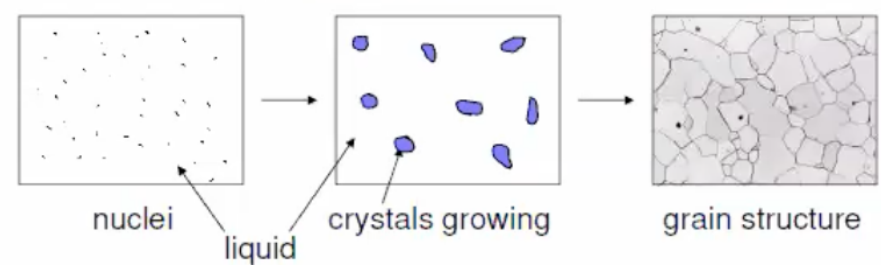
θ_c = critical angle

2.4 Imperfections and Diffusion

2.4.1 Solidification

Nucleation: Nuclei of solid form in liquid

Growth: Nuclei grow to form crystals – crystals grow until all liquid consumed leaving grains



Grain types:

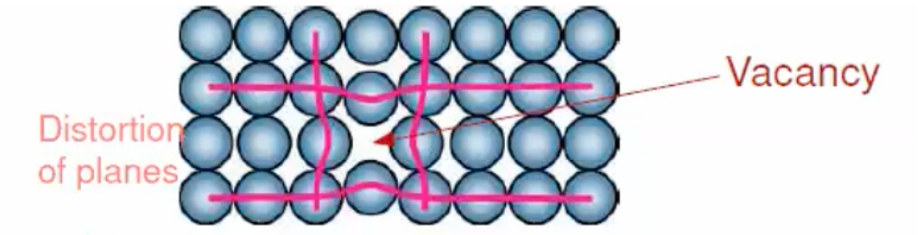
1. Equiaxed: Same size in all directions
2. Columnar: Elongated

2.4.2 Imperfections

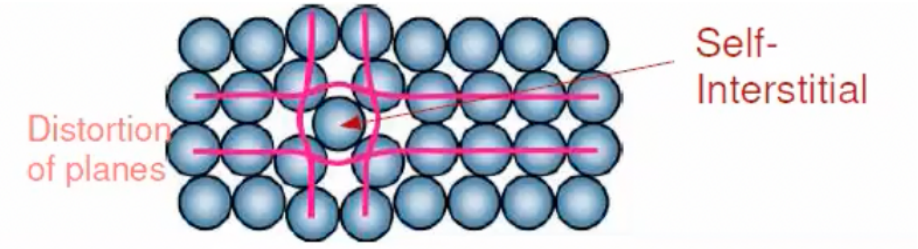
Types of Imperfections:

1. Point Defects
   - Vacancies
   - Interstitial Atoms
   - Substitutional Atoms
2. Line Defects
   - Dislocations
3. Areal Defects
   - Grain boundaries

Vacancy:



Interstitial Atoms



$$\frac{N_v}{N} = e^{\frac{-Q_v}{kT}} \tag{86}$$

$$k = 1.38 \times 10^{-23} \frac{J}{atom \cdot K} = 8.62 \times 10^{-5} \frac{eV}{atom \cdot K} \tag{87}$$

$$N = \rho V \frac{N_A}{A} \tag{88}$$

N_v = No. of Defects

N = No. of potential defect sites

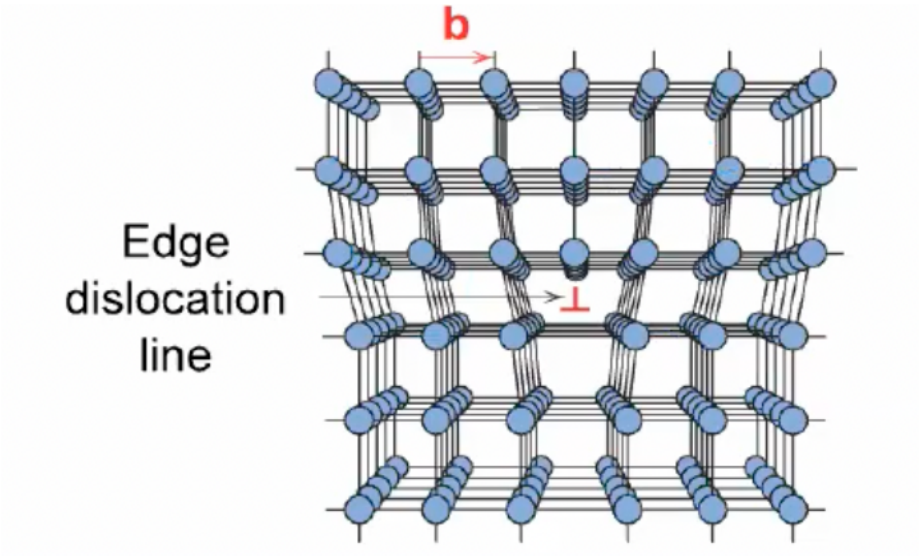
Q_v = Activation Energy

Conditions for substitutional solid solutions: Hume – Rothery rules

1. $\Delta r < 15\%$
2. Proximity in periodic table (Low ΔE)
3. Same crystal structure for pure metals
4. Valency

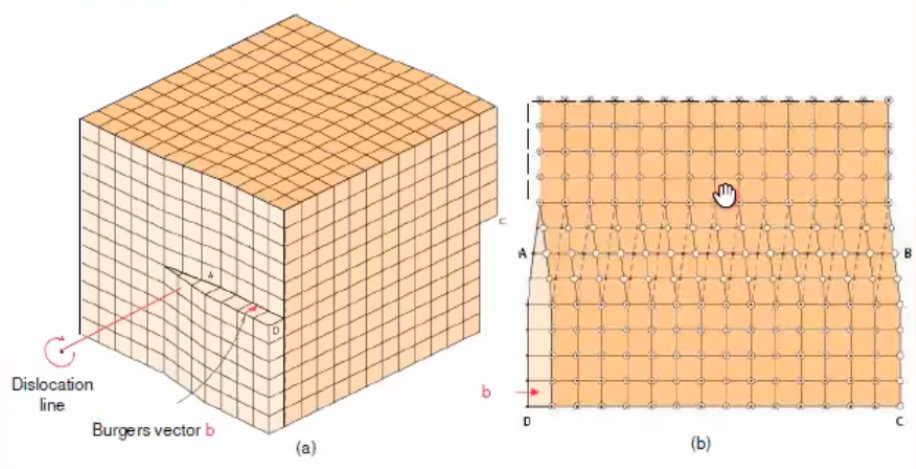
Edge Dislocations

1. Extra half plane inserted into a crystal structure
2. Burgers Vector, b is perpendicular $\perp$ to the dislocation line



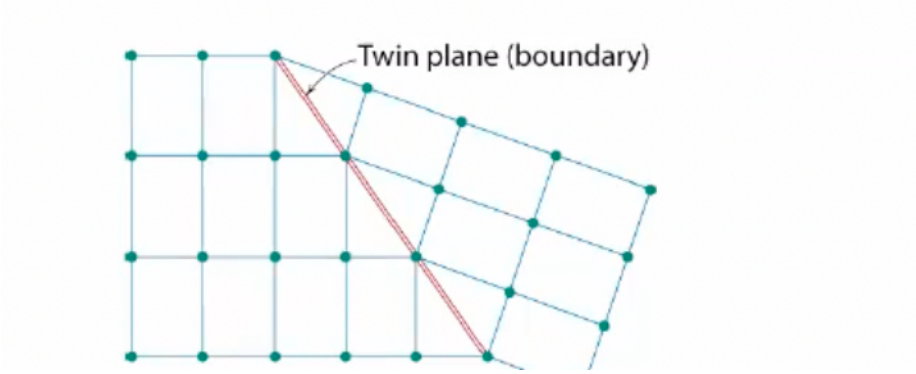
Screw Dislocations

1. spiral planar ramp resulting from shear deformation
2. b is parallel || to dislocation line



Twin boundary (plane)

1. Relfection of atom positions across the twin plane



Staking Faults

1. For FCC – An error in ABc packing sequence
2. e.g. ABCABCABC → ABCABABC

2.5 Diffusion

Inter-Diffusion: In an alloy, atoms migrate from regions of high concentration to regions of low concentration

Self-Diffusion: In an elemental solid, atoms migrate

Vacancy Diffusion: Atoms exchange vacancies. The rate depends on the concentration of vacancies and the activation energy for an exchange

Intersitial Diffusion: Smaller atoms diffuse between host attoms. This happens more rapidly than vacancy diffusion because they aren't strongly

2.5.1 Time independant

$$J = \frac{M}{At} = \frac{1}{A}\frac{dM}{dt} \tag{89}$$

$$J = -D\frac{dC}{dx} \tag{90}$$

$$\text{If linear } \frac{dC}{dx} \cong \frac{\Delta C}{\Delta x} = \frac{C_2 - C_1}{x_2 - x_2} \tag{91}$$

$$D = D_0 \cdot e^{-\frac{Q_d}{RT}} \tag{92}$$

$$\tag{93}$$

2.5.2 Non Steady State Diffusion

$$\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2} \tag{94}$$

$$\frac{C(x,t) - C_0}{C_s - C_0} = 1 - erf\left(\frac{x}{s\sqrt{Dt}}\right), \text{ where: } erf(z) = \frac{2}{\sqrt{\pi}}\int_0^z e^{-y^2}dy \tag{95}$$

3 Phase diagrams