

1 Atomic Structure

1.1 Energy

$$u_v dv = \frac{8\pi v^2}{c^3} \cdot \frac{hv}{e^{\frac{hv}{k_b T}} - 1} \quad (1)$$

$$E = hv \quad (2)$$

1.2 Photoelectric Effect

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

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

$$R_H = 1.097373 \times 10^7 m^{-1} \quad (5)$$

$$n_1 = 1 \Rightarrow \textit{Lyman} \quad (6)$$

$$n_1 = 2 \Rightarrow \textit{Balmer} \quad (7)$$

$$n_1 = 3 \Rightarrow \textit{Paschen} \quad (8)$$

$$n_1 = 4 \Rightarrow \textit{Brackett} \quad (9)$$

$$n_1 = 5 \Rightarrow \textit{Pfund} \quad (10)$$

$$n_2 > n_1 \quad (11)$$

1.3 De Broglie Relationship

$$E^2 = p^2 c^2 + m^2 c^4 \quad (12)$$

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

$$hv = h \frac{c}{\lambda} = pc \quad (14)$$

$$\therefore p = \frac{h}{\lambda} \quad (15)$$

1.4 Electron diffraction

$$E_K = eV - \frac{p^2}{2m} \quad (16)$$

$$p = \sqrt{2meV} \quad (17)$$

$$\lambda = \frac{h}{\sqrt{2meV}} \quad (18)$$

$$\lambda = 2d \sin(\theta) \quad (19)$$

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

1.5 Bohr Model

$$F_{centripetal} = F_{electric} \quad (21)$$

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

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

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

$$\therefore v = \frac{hn}{2\pi mr} \quad (25)$$

$$L = mvr = n \frac{h}{2\pi} = n\hbar \quad (26)$$

$$\text{As such, allowed radii are described by the expression:} \quad (27)$$

$$r_n = \frac{h^2\epsilon_0 n^2}{\pi m e^2} = a_{Bohr} n^2 \quad (28)$$

$$r_1 = a_{Bohr} = \frac{h^2\epsilon_0}{\pi m e^2} = 5.3 \times 10^{-11} m \quad (29)$$

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

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

$$\text{Substituting in } r_n \text{ gives:} \quad (32)$$

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

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

$$\text{since: } E = hv = h \frac{c}{\lambda} \quad (35)$$

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

1.6 Waves

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

$$k = 2\pi/\lambda \quad (38)$$

$$\omega = 2\pi v \quad (39)$$

$$c = v\lambda = \frac{\omega}{2\pi} \cdot \lambda = \frac{\omega}{\lambda} \quad (40)$$

$$P(x) \propto |\Psi|^2 dx \quad (41)$$

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

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

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

$$\text{Einstein: } E = hv = h\frac{\omega}{2\pi} = \hbar\omega \quad (45)$$

$$\frac{\partial}{\partial x}\Psi = i\frac{p}{\hbar}\Psi \Rightarrow p\Psi = \{-i\hbar\frac{\partial}{\partial x}\}\Psi \quad (46)$$

$$\frac{\partial}{\partial t}\Psi = -i\frac{E}{\hbar}\Psi \Rightarrow E\Psi = \{i\hbar\frac{\partial}{\partial t}\}\Psi \quad (47)$$

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

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

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

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

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

1.8 Time independent Shrodinger's Equation

$$\Psi(x, t) = \phi(t)\psi(x) \quad (52)$$

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

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

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

$$\text{By unit analysis: } A = E \quad (56)$$

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

1.9 Electron in a box

$$V(0) = V(L) = \inf \quad (58)$$

$$V(x) = 0 \quad \forall x \mid 0 < x < L \quad (59)$$

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

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

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

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

$$E = \frac{\hbar^2 k^2}{2m} \quad (64)$$

$$\text{Applying boundary conditions:} \quad (65)$$

$$\psi(0) = 0 \Rightarrow B = 0 \quad (66)$$

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

$$\therefore kL = n\pi, \quad n = 1, 2, 3, \dots \quad (68)$$

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

$$E_n = \frac{\hbar^2}{8mL^2} \cdot n^2 \quad (70)$$

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

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

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

1.10 3D

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

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

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

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

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

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

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

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

2 Bonding and Crystalline Structure

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

2.1 I don't have a good title yet

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

$$\text{ionic character} = 1 - e^{-\frac{(x_A - x_B)^2}{4}} \quad (78)$$

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

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

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

$$\rho = \frac{nA}{V_c N_a} \quad (81)$$

$$LD = \frac{n_a}{r} \quad (82)$$

$$PD = \frac{n}{a^2} \quad (83)$$

2.3 X-Ray Diffraction

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

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

d = planar spacing

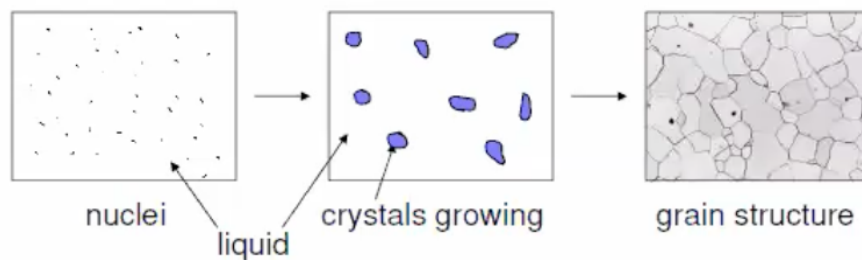
θ_c = critical angle

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

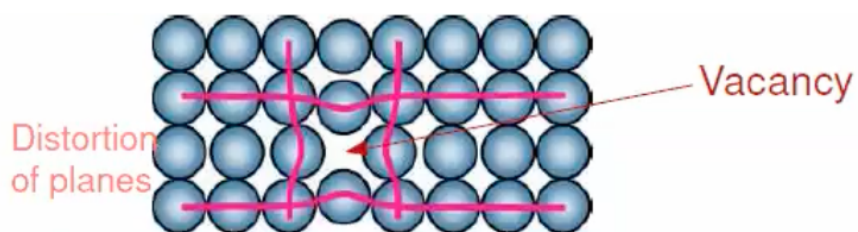
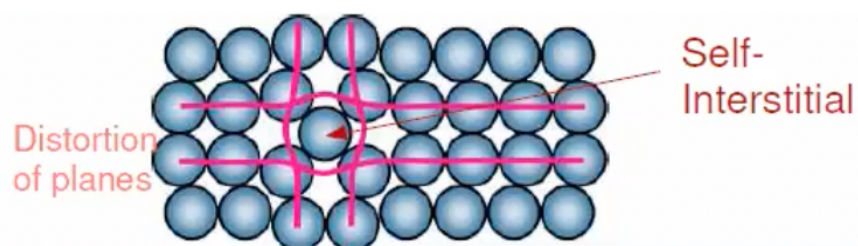


Grain types:

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**

$$\frac{N_v}{N} = e^{\frac{-Q_v}{kT}} \quad (86)$$

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

$$N = \rho V \frac{N_A}{A} \quad (88)$$

N_v = No. of Defects

N = No. of potential defect sites

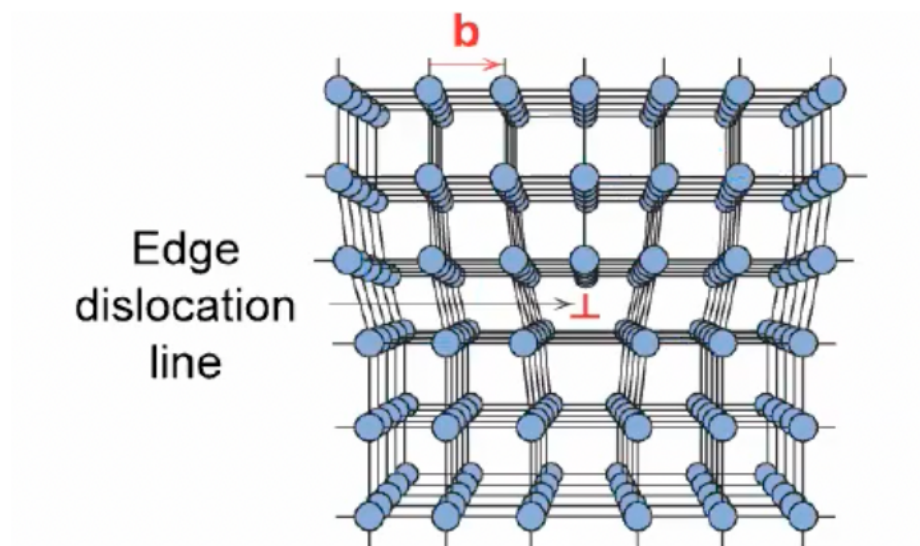
Q_v = Activation Energy

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

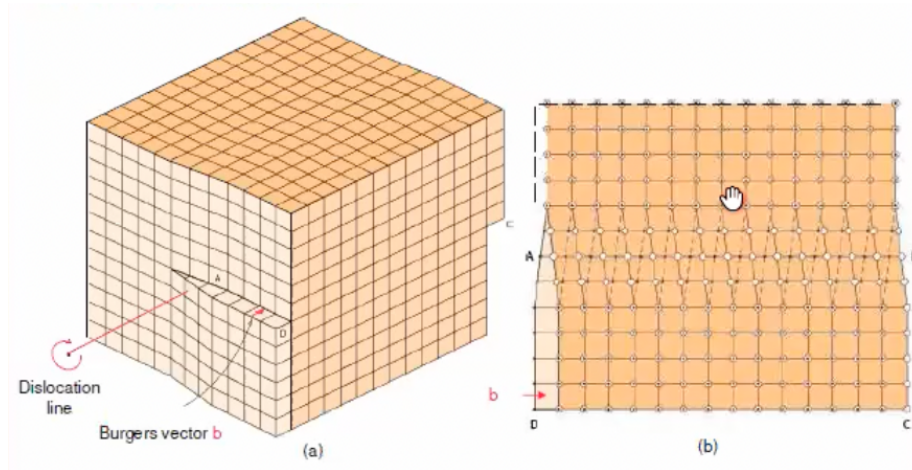
Edge Dislocations

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



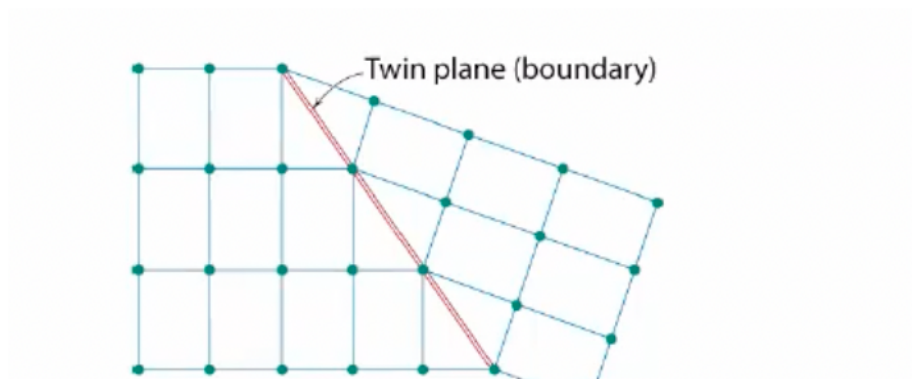
Screw Dislocations

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



Twin boundary (plane)

1. Reflection of atom positions across the twin plane



Stacking Faults

1. For FCC – An error in ABc packing sequence
2. e.g. ABCABCABC \rightarrow 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

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

2.5.1 Time independant

$$J = \frac{M}{At} = \frac{1}{A} \frac{dM}{dt} \quad (89)$$

$$J = -D \frac{dC}{dx} \quad (90)$$

$$\text{If linear } \frac{dC}{dx} \cong \frac{\Delta C}{\Delta x} = \frac{C_2 - C_1}{x_2 - x_1} \quad (91)$$

$$D = D_0 \cdot e^{-\frac{Q_d}{RT}} \quad (92)$$

$$(93)$$

2.5.2 Non Steady State Diffusion

$$\frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2} \quad (94)$$

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

3 Phase diagrams

Lever Rule

$$M_{\alpha} \times S = M_L \times R \quad (96)$$

$$W_L = \frac{M_L}{M_L + M_{\alpha}} = \frac{S}{R + S} = \frac{C_{\alpha} - C_0}{C_{\alpha} - C_L} \quad (97)$$

$$W_{\alpha} = \frac{R}{R + S} = \frac{C_0 - C_L}{C_{\alpha} - C_L} \quad (98)$$

