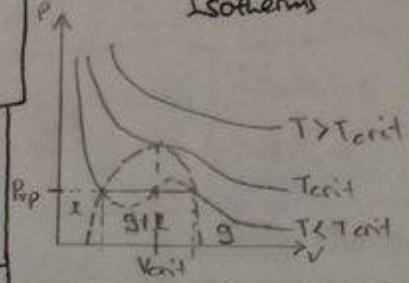
Properties of Matter Cheat Sheet

Van der Waals eqⁿ

$$\left(P + \frac{an^2}{V^2}\right)(V - nb) = nRT$$

Van der Waals Isotherms



$V_{crit} = 3b$

$P_{crit} = \frac{a}{27b^2}$

$T_{crit} = \frac{8a}{27bR}$

T > Tcrit no liquid phase (super critical fluid)

Work Done (isothermic)

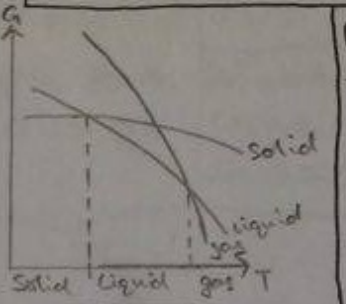
$$W = -\int P\,dV = -\int \frac{nRT}{V-nb} - \frac{an^2}{V^2}\,dV$$

Gibbs free energy @ transitions.

$G = U + PV - TS$

$$L = \Delta S\, T_t$$

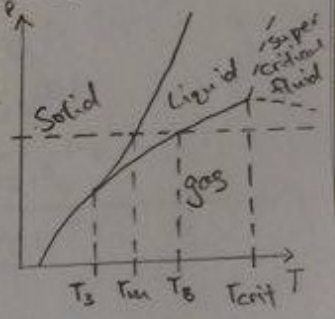
L = latent heat, ΔS = change in entropy, T_t = transition temp



Phase Diagrams

T_{triple} - 3 phases in equilibrium

$G_l = G_g = G_s$



Clapeyron Equation

$$\frac{dP}{dT} = \frac{\Delta S}{\Delta V} = \frac{L}{T\Delta V}$$

Coulomb Potential

$$V(r) = \frac{-q^2}{4\pi\varepsilon_0 r} + \frac{A}{r^{12}}$$

$$r_0 = \left[\frac{98A\pi\varepsilon_0}{q^2}\right]^{1/11}$$

Bond Comparison

	Lennard Jones	Coulomb	Morse
Range	quite short	Long	very short
Type of bond	molecular	ionic crystals	covalent crystal, lattice
Eg.	Solid CO_2	NaCl Crystals	Diamond

Lennard Jones Potential

$$V(r) = -4\varepsilon\left[\left(\frac{\sigma}{r}\right)^6 - \left(\frac{\sigma}{r}\right)^{12}\right]$$

$r_0 = 2^{\frac{1}{6}}\sigma$ (no vibrations)

$V(r)$ @ $r_0 = -\varepsilon$

Morse Potential

$$V(r) = D\left[e^{-2a(r-r_0)} - 2e^{-a(r-r_0)}\right]$$

$V(r_0) = -D$

Thermal expansion

$$\frac{\Delta l}{l} = \alpha \Delta T$$

α → thermal expansion coefficient

For $V(r_0) \leq V < 0$ the particles vibrate between 2 radii, r_1 & r_2

Bond length = $r_{avg} = \frac{r_1 + r_2}{2} > r_0$

Cohesive Energy

$$E_{COH} = -U_{pot} = \frac{1}{2}\sum_{i,j=1}^{N} V(r_{ij})$$

Coulomb pot: $E_{COH} = -\frac{q^2}{4\pi\varepsilon_0 r_0}\ln 2$

Morse pot.: E_{COH} use only 1st nearest neighbour

Young's Modulus (E)

$$E = \frac{\text{tensile Stress}}{\text{Strain}} = \frac{\sigma}{\varepsilon}$$

$$E = -\frac{1}{r_0}\left.\frac{d^2V}{dr^2}\right|_{r_0}$$

Miller indices

- describes a plane with lattice vectors $\vec{a_1}, \vec{a_2}$ and $\vec{a_3}$ (need not be orthogonal).
- Miller indices = (h k l)

$\vec{A_1} = \frac{1}{h}\vec{a_1}$

$\vec{A_2} = \frac{1}{k}\vec{a_2}$

$\vec{A_3} = \frac{1}{l}\vec{a_3}$

FCC

- 8 corner atoms
- 6 central atoms
- Atoms per cell = 4

$a = 2\sqrt{2}\,r$

a = length of cell, r = radius of atom

ABCABC stacking

Packing Fraction

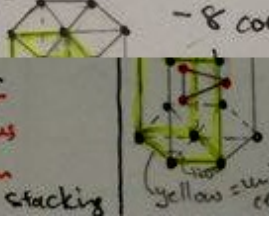
$$= \frac{\text{volume of atoms}}{\text{volume of unit cell}}$$

BCC

- 8 corner atoms
- 1 central atoms
- Atoms per cell = 2

$a = \frac{4}{\sqrt{3}}r$ ← atomic radius

HCP



Similar to BCC*

- 8 corner atoms
- 1 central atom
- Atoms per cell = $\frac{7}{3}$

Stacking: AB AB AB