Solid State Physics

Three phases of matter

1. Solid
2. Liquid
3. Gas

} Important difference: difference of structure

Solids & liquids have nearly same density.

Solids have structure (energetically favoured)

Crystalline solids → Long-range order

Polycrystalline.

Amorphous solids → short-range order

(Eg. glass, tar). [like high-viscosity liquids]

Bonds vary in strength, leading causes gradual breaking of structure.

Crystalline solids :

1. Fracture dynamics and presence of defects.
2. Energetically more favourable configuration.

Ionic crystals (ionic bonding)

Ionic Bonds are formed:

1/ Atoms with low ionization energy give up an electron.

2/ Atoms with high electron affinity pick up an electron.

3/ An ion is surrounded by oppositely charged ions as closely as possible. Ordered structure.

4. Total energy is less compared to the ~~for~~ total energy of free atoms.

Cohesive Energy: Energy per ion needed to separate the components into neutral free atoms.

Lattice Energy: Energy per ion needed to separate the components into free ions.

Covalent bonding

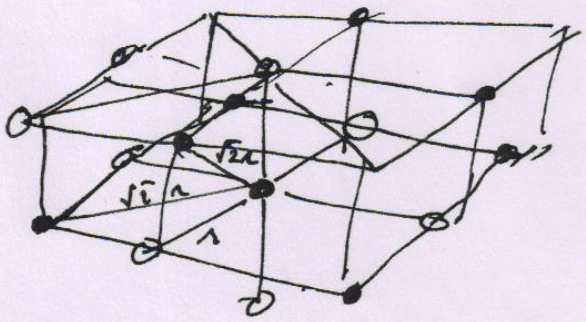
1. Sharing of an electron (localised in the region between two atoms).
2. Strong directional properties. Eg. graphite (variety).
3. Can work for both atoms (carbon, silicon) and molecules (molecular hydrogen)
4. Cohesive energies are higher usually, compared to ionic crystals.

Metallic bonding

1. Valence electrons in atoms form an electron gas.
2. The electrons move freely.
3. An electron is closer to an ion in this arrangement. So energetically favourable.
4. Electrons have higher kinetic energy, and form a continuous energy band.

(Pauli's exclusion principle, Heisenberg's Uncertainty Principle).

Ionic bonding:



A central Na^+ ion has 6 Cl^- nearest neighbours.

$$U(r) = -\frac{6e^2}{4\pi\epsilon_0 r}$$

Next-nearest neighbours are 12 Na^+ ions.

$$U(r) = \frac{e^2}{4\pi\epsilon_0 r} \cdot \frac{12}{\sqrt{2}}$$

$$U_{Coulomb} = -\frac{e^2}{4\pi\epsilon_0 r}\left[6 - \frac{12}{\sqrt{2}} + \cdots\right]$$

$$= -\frac{\alpha e^2}{4\pi\epsilon_0 r}$$

$\alpha \longrightarrow$ Madelung Constant.

$1.6 < \alpha < 1.8$

1. Dependent on the lattice structure
2. Represents an overall effect of the total electric field of all particles.

Repulsive Potential : (Max Born)

$$U_{repulsive} = \frac{B}{r^n}$$

n is typically large
$n \gg 1$, $n \sim 10$

1. Pauli's Exclusion Principle.
2. Short range repulsive force.
3. Very weak at large distances.

$$U_{total} = U_{coulomb} + U_{repulsive}$$

$$U(r) = \frac{-\alpha e^2}{4\pi\epsilon_0 r} + \frac{B}{r^n}$$

At $r = r_0$ (Equilibrium position)

$$\frac{dU}{dr} = 0 \Rightarrow -\frac{\alpha e^2}{4\pi\epsilon_0} \times \frac{-1}{r^2} + B \times \frac{-n}{r^{n+1}} = 0$$

$$\Rightarrow \frac{\alpha e^2}{4\pi\epsilon_0 r_0^2} - \frac{nB}{r_0^{n+1}} = 0$$

$$\Rightarrow B = \frac{\alpha e^2}{4\pi\epsilon_0 r_0^2} \cdot \frac{1}{n} r_0^{n+1}$$

$$\Rightarrow B = \frac{\alpha e^2}{4\pi\epsilon_0} \cdot \frac{1}{n} r_0^{n-1}$$

$$U(r) = -\frac{\alpha e^2}{4\pi\epsilon_0}\cdot\frac{1}{r} + \frac{\alpha e^2}{4\pi\epsilon_0}\cdot\frac{1}{n}\left(\frac{r_0}{r}\right)^n \cdot \frac{1}{r_0}$$

$$U(r) = -\frac{\alpha e^2}{4\pi\epsilon_0}\left[\frac{1}{r} - \frac{1}{n}\left(\frac{r_0}{r}\right)^n \frac{1}{r_0}\right]$$

When $r = r_0$.

$$U(r_0) = -\frac{\alpha e^2}{4\pi\epsilon_0}\cdot\frac{1}{r_0}\left[1 - \frac{1}{n}\right]$$

Cohesive Energy → $U(r_0)$ +

Energy needed to return the electrons to the ions.

$n \simeq 9$. (High repulsion)

Ex. 10.1 (B-eisen)

Interatomic Potentials :

$$U(r) = -\frac{A}{r^m} + \frac{B}{r^n}$$

$n > m$, $n, m > 0$

For van der Waal's bonding

$m = 6$.

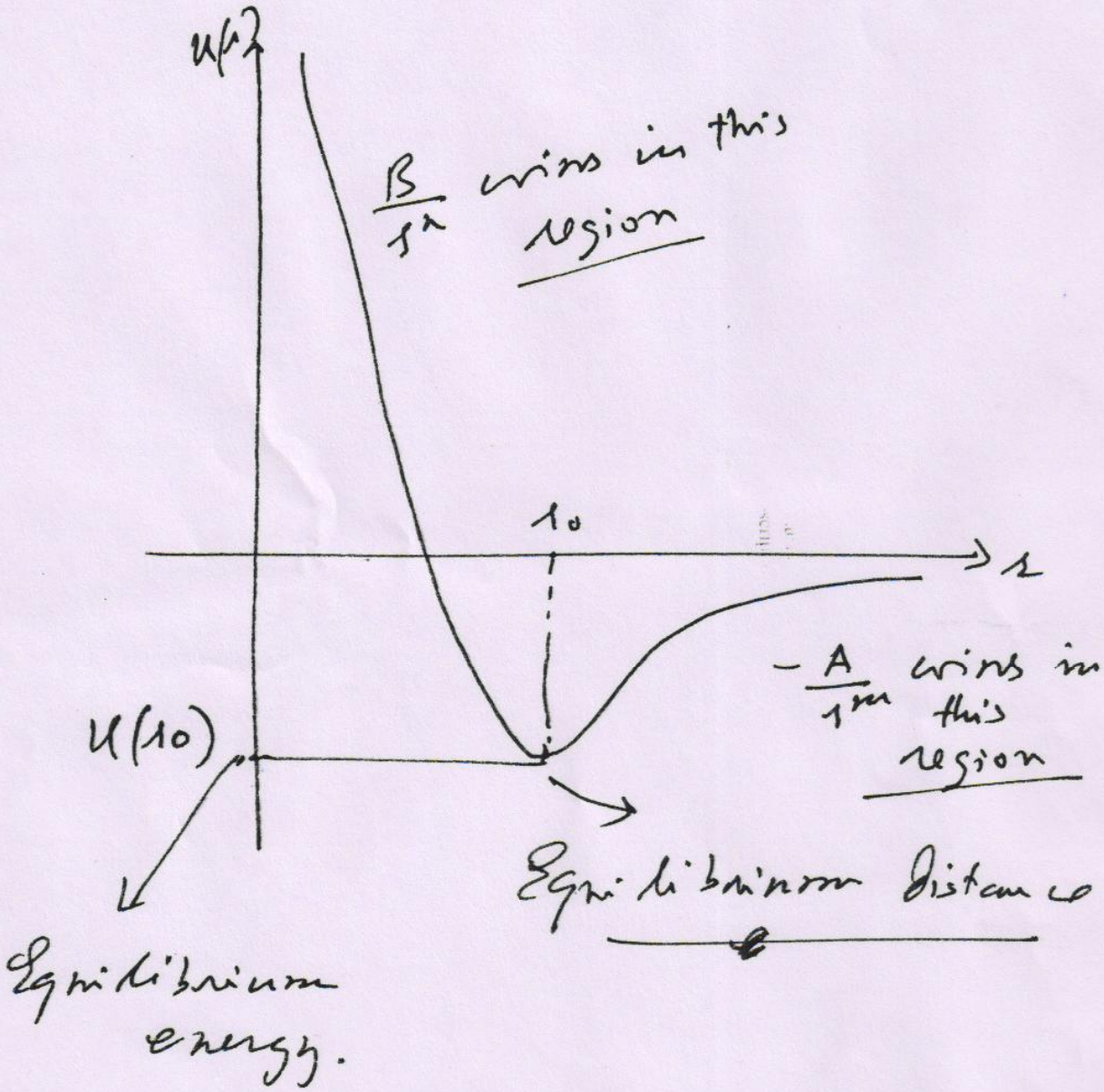
when $n = 12$, → Lennard-Jones potential.

For ionic bonding $m = 1$.

At equilibrium, $\frac{dU}{dr} = 0$.

$r = r_0$ equilibrium separation

$U(r_0)$ → (Equilibrium energy or stable energy)



$$U(r) \equiv -\frac{A}{r^m} + \frac{B}{r^n}$$