LECTURE 1
INTERATOMIC FORCES

(Solid State physics S.O.Pillai)

http://202.141.40.218/wiki/index.php/
Unit-3:_Atomic_Cohesion_and_Crystal_Binding#FORCE_BETWEEN_ATOMS

Matter:

- *Solid State*
- *Liquid State*
- *Gaseous State*
- *Plasma (99% of universe)*
  - Few centuries ago: few metals/alloys
  - Since last century: a large no. of new materials/crystal/alloys
  - Different physical/chemical/electrical properties ??

Solid/crystal ⟶ *Molecules* ⟶ *Atoms* ⟶ *Basic Particles*

- physical/chemical/electrical properties depends on
  - Arrangement and interaction of atoms/molecules
  - Definite pattern governed by bonding
  - Bonding is governed by interaction

Q: What kind of force holds the atoms together in solid?

The bonds are made of attractive and repulsive forces that tend to hold the adjacent atoms, this process of holding atoms together is known as ***BONDING****.*

Interatomic Binding

- *All of the mechanisms which cause bonding between the atoms derive from electrostatic interaction between nuclei and electrons. Magnetic interaction is weak and gravitational is negligible*

- *The differing strengths and differing types of bond are determined by the particular electronic structures of the atoms involved.*

- *Type of Bonding decides the physical, chemical and electrical properties .*

- *Bonds are made due to the resultant force of attraction and repulsion b/w atoms.*

- *This force hold the adjacent atoms together at particular spacing/position/pattern.*

Forces Between Atoms

Forces between atoms → Attractive (keep the atoms together)

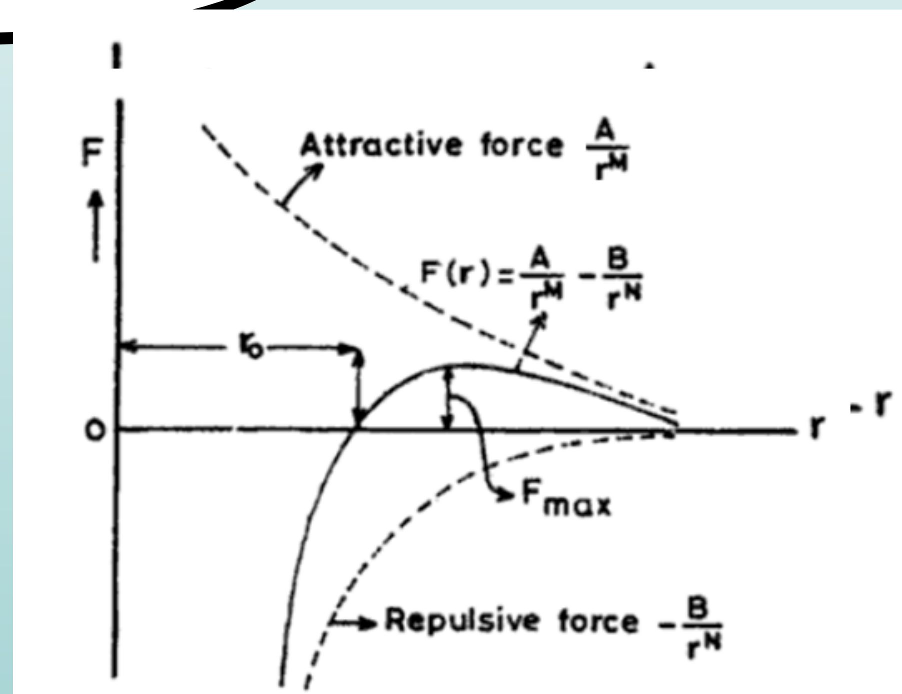
→Repulsive (when solid is compressed)

Suppose two atoms, exert attractive and repulsive forces on each other such that the bonding force is

Due to attractive force

Due to repulsive force

$$F(r) = \frac{A}{r^M} - \frac{B}{r^N} \quad \text{with } N>M$$



Where, r→ centre to centre spacing between the atoms.

A, B, M and N are constants characteristics of the molecule.

At equilibrium, when $r=r_o$
$F(r)=0$
Thus,

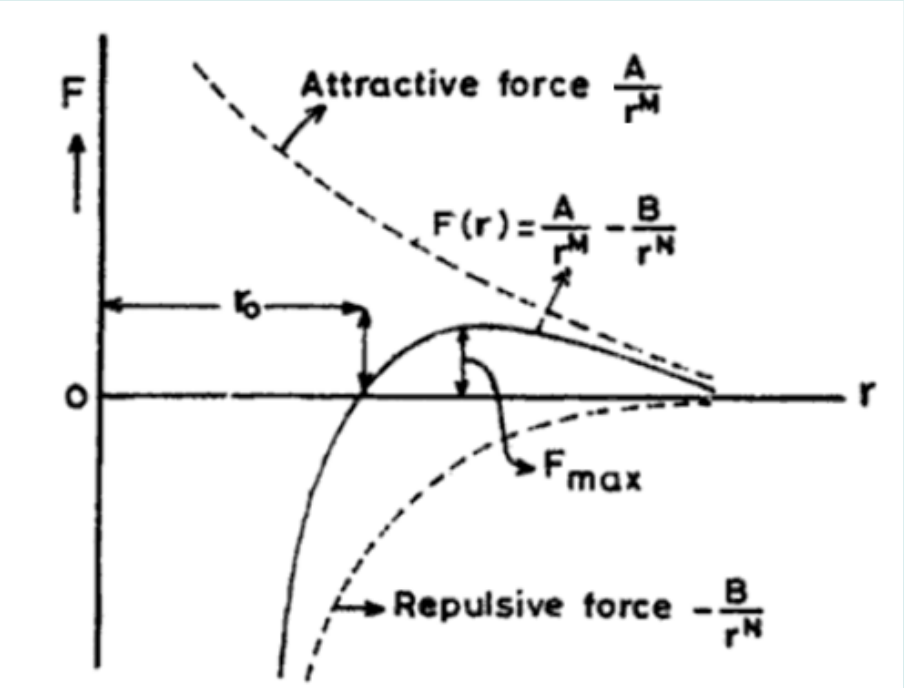
$$\frac{A}{r^M} - \frac{B}{r^N} = 0$$

$$\Rightarrow \frac{A}{r^M} = \frac{B}{r^N}$$

$$\Rightarrow r_o^{N-M} = \frac{B}{A}$$

$$\boxed{F(r) = \frac{A}{r^M} - \frac{B}{r^N} \quad \text{with} \quad N>M}$$

$$\boxed{r_o = \left(\frac{B}{A}\right)^{\frac{1}{N-M}}}$$



Potential Energy

$$F(r) = \frac{A}{r^M} - \frac{B}{r^N}$$

Thus,

$$U(r) = \int F(r)dr = \int \left(\frac{A}{r^M} - \frac{B}{r^N}\right)dr$$

$$= \frac{Ar^{1-M}}{1-M} - \frac{Br^{1-N}}{1-N} + C$$

$$U(r) = -\frac{a}{r^m} + \frac{b}{r^n} + C$$

where $a = \dfrac{A}{M-1}$, $b = \dfrac{B}{N-1}$, m=M-1, n=N-1

U=0 when r=∞ ⇒ C=0 and

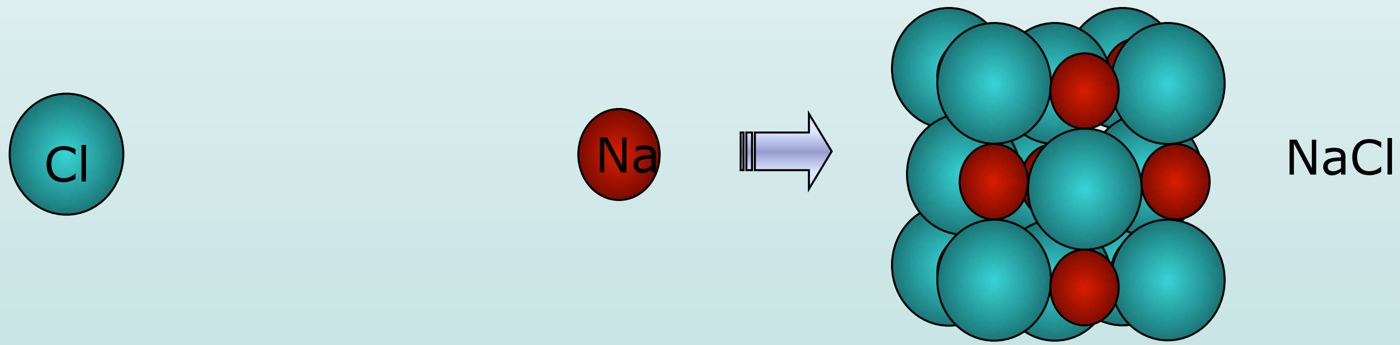
$$\boxed{U(r) = -\frac{a}{r^m} + \frac{b}{r^n}}$$

r : distance between the centers of the atoms
n and m are +ve numbers
a: +ve constant
b: +ve constant

- *Potential energy due to attraction is –ve , since the atoms do the work of attraction.*
- *Potential energy due to repulsion, energy is +ve, since external work must be done to bring the atoms together*
- *Potential energy is inversely proportional to some power of inter-atomic spacing 'r'.*

Energies of Interactions Between Atoms

- *The energy of the crystal is **lower** than that of the free atoms by an amount equal to the energy required to pull the crystal apart into a set of free atoms. This is called the binding (cohesive) energy of the crystal.*
  - *NaCl is more stable than a collection of free Na and Cl.*



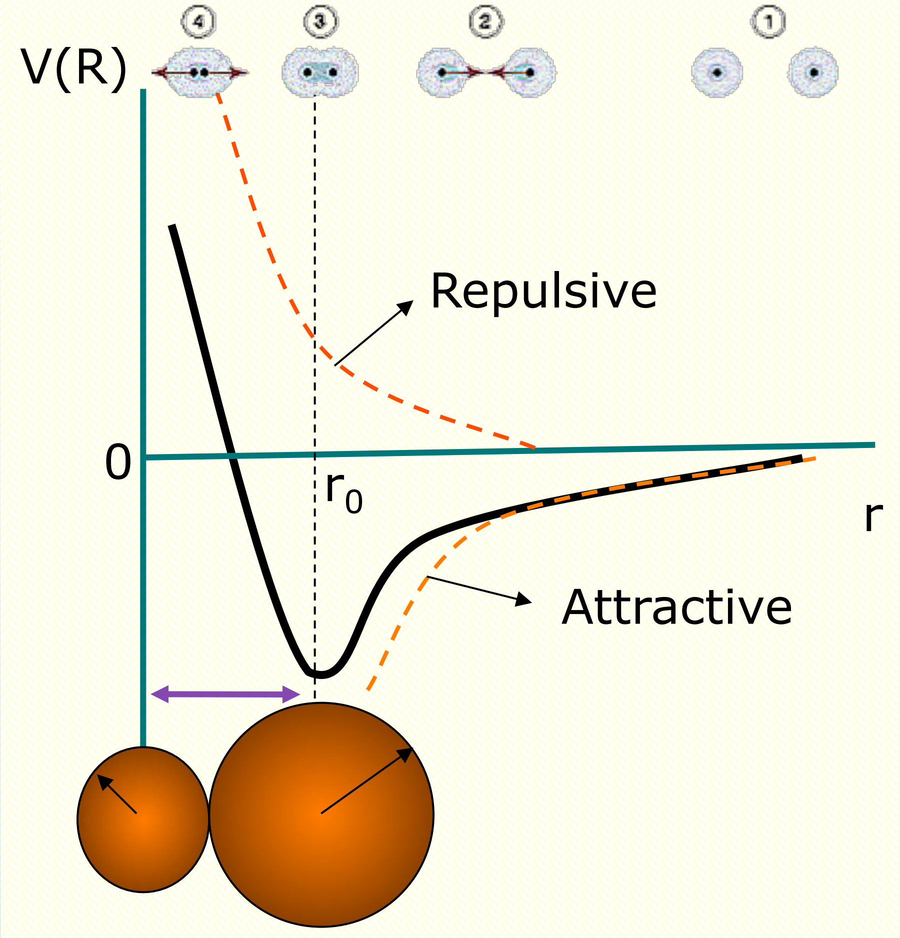
The potential energy of either atom will be given by:

U= decrease in potential energy+increase in potential energy
(due to attraction) **(due to repulsion)**

or simply:

$$U(r) = \frac{-a}{r^m} + \frac{b}{r^n}$$

- This typical curve has a minimum at equilibrium distance r_0
- $r > r_0$;
  - the potential increases gradually, approaching 0 as $R \rightarrow \infty$
  - the force is attractive
- $r < r_0$;
  - the potential increases very rapidly, approaching ∞ at small separation.
  - the force is repulsive



- At equlibrium, repulsive force becomes equals to the attractive part.

The potential energy of either atom will be given by:

- Potential Energy Curve

or simply:

$$U(r) = \frac{-a}{r^m} + \frac{b}{r^n}$$

- Quest: Determine U_{min}, value of $r = r_0$=?

Potential Energy → Cohesive Energy

The energy corresponding to the equilibrium position ($r=r_o$) denoted by $U(r_o)$ is called **the bonding energy or the energy of cohesion** of the molecule. This is the energy required to dissociate the two atoms of the molecule (AB) into an infinite separation. This energy is also known as ***the energy of dissociation***.

$$U(r) = -\frac{a}{r^m} + \frac{b}{r^n}$$

U(r) is mimimum at $r=r_o$

$$\text{Thus , } U(r) = -\frac{a}{r_o^m} + \frac{b}{r_o^n}$$

$$\text{Hence, } \left[\frac{dU}{dr}\right]_{r=r_o} = \frac{ma}{r_o^{m+1}} - \frac{nb}{r_o^{n+1}} = 0$$

$$r_o^n = r_o^m\left[\left(\frac{b}{a}\right)\left(\frac{n}{m}\right)\right]$$

$$U_{min} = -\frac{a}{r_o^m} + b\left(\frac{a}{b}\right)\left(\frac{m}{n}\right)\frac{1}{r_o^m}$$

$$U_{min} = \frac{a}{r_o^m}\left(\frac{m}{n}\right) - \left[\frac{a}{r_o^m}\right]$$

$$\boxed{U_{min} = -\frac{a}{r_o^m}\left(1 - \frac{m}{n}\right)}$$

Potential Energy

Let r_o be the distance between the atoms for this minimum U(r) to occur.

$r_o \rightarrow$ equillibrium spacing of the system. ***$U(r=r_o)_{min} \rightarrow -ve$***

$$U(r) = -\frac{a}{r^m} + \frac{b}{r^n}$$

U(r) is mimimum at $r=r_o$

$$\text{Thus ,} \left[\frac{dU}{dr}\right]_{r=r_o} = 0$$

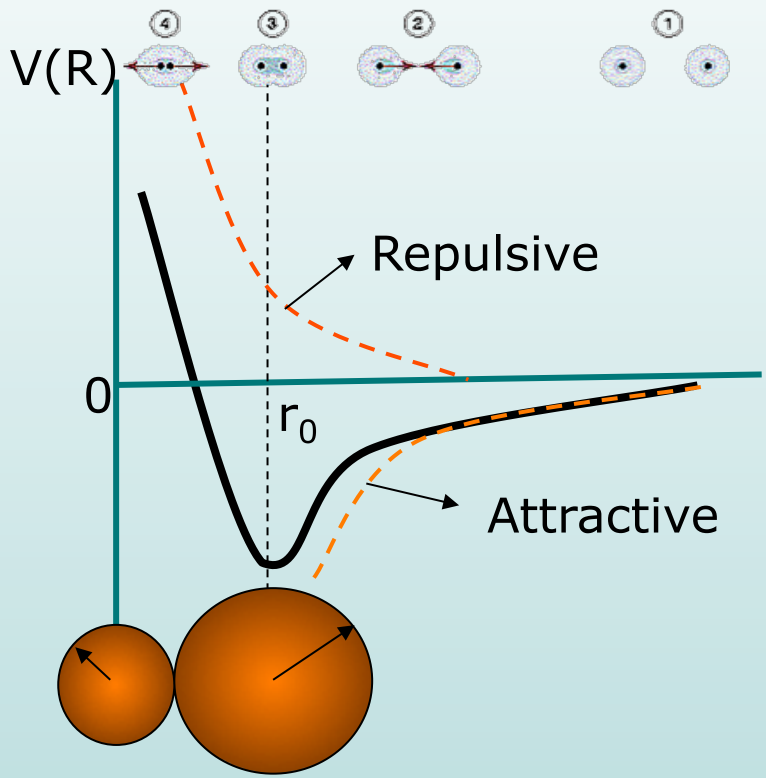
$$\boxed{r_o = \left[\left(\frac{b}{a}\right)\left(\frac{n}{m}\right)\right]^{\frac{1}{n-m}}}$$

$$\left[\frac{d^2U}{dr^2}\right]_{r=r_o} = -\frac{am(m+1)}{r_o^{m+2}} + \frac{bn(n+1)}{r_o^{n+2}} > 0$$

$$bn(n+1) > am(m+1)r_o^{n-m}$$

$$bn(n+1) > am(m+1)\left(\frac{b}{a}\right)\left(\frac{n}{m}\right)$$

$$\boxed{\begin{array}{c}(n+1) > (m+1) \\ n > m\end{array}}$$



The minimum for U(r) occur only if

n > m

$\Rightarrow$ The attractive force should vary more slowly with r than repulsive force.

Problem: 1

- Given Potential energy function is $U(r) = -\frac{a}{r} + \frac{b}{r^9} \ldots$

(a) Show that $r = r_o = \left[\frac{9b}{a}\right]^{1/8}$ in stable situation

(b) Show that potential energy of the two particles in the stable configuration is

$$U(r)_{min} = -\left[\frac{a}{r_o}\right]\left[\frac{8}{9}\right]$$

Problem:2

Assume the energy of two particles in the field of each other is given by the following function of the distance 'r' between the centers of the particles:

$$U(r) = -\frac{a}{r} + \frac{b}{r^8}$$

a)Show that the two particles from a stable compound for

$$r = r_o = \left[\frac{8b}{a}\right]^{1/7}$$

b)Show that the P.E. of the two particles in the stable configuration is equal to

$$-\left[\frac{7}{8}\right](a / r_o)$$

c)Show that if the particles are pulled apart, the molecule will break a soon as

$$r = \left[\frac{36b}{a}\right]^{1/7}$$

and that the minimum force required to break the molecule is

$$\frac{a^{9/7}}{(36b)^{2/7}}\left[1 - \frac{8}{36}\right]$$

Example S1

The potential energy function for the force between two particular ions, carrying charges $+e$ and $-e$ respectively, may be written as,

$$V = -\frac{Ae^2}{r} + \frac{B}{r^9}$$

(i) Find the equilibrium separation distance for these ions.

(ii) Find the potential energy at equilibrium separation.

At equilibrium separation, r_o the cohesive force between the ions drops to zero.

$$V = -\frac{Ae^2}{r} + \frac{B}{r^9}$$

$$\left.\frac{dV}{dr}\right|_{r=r_0} = 0$$

$$-\frac{Ae^2}{r_0^2} + \frac{9B}{r_0^{10}} = 0$$

$$r_0^8 = \frac{9B}{Ae^2}$$

$$r_0 = \left(\frac{9B}{Ae^2}\right)^{\frac{1}{8}}$$

The ratio B/A is the dominating factor.

Substituting this value of r_o back into the potential energy function gives:

$$
\begin{aligned}
V(r_o) &= -\frac{Ae^2}{r_o} + \frac{B}{r_o^{\,9}} \\
&= -\frac{1}{r_o}\left(Ae^2 - \frac{B}{r_o^{\,8}}\right) \\
&= -\frac{1}{r_o}\left[Ae^2 - B\left(\frac{Ae^2}{9B}\right)\right] \\
&= -\frac{1}{r_o}\left(\frac{8Ae^2}{9}\right) \\
&= -\left(\frac{Ae^2}{9B}\right)^{\frac{1}{8}}\left(\frac{8Ae^2}{9}\right)
\end{aligned}
$$

The constant A should dominate over the 8th root.