Crystal Binding
(Solid State Physics)

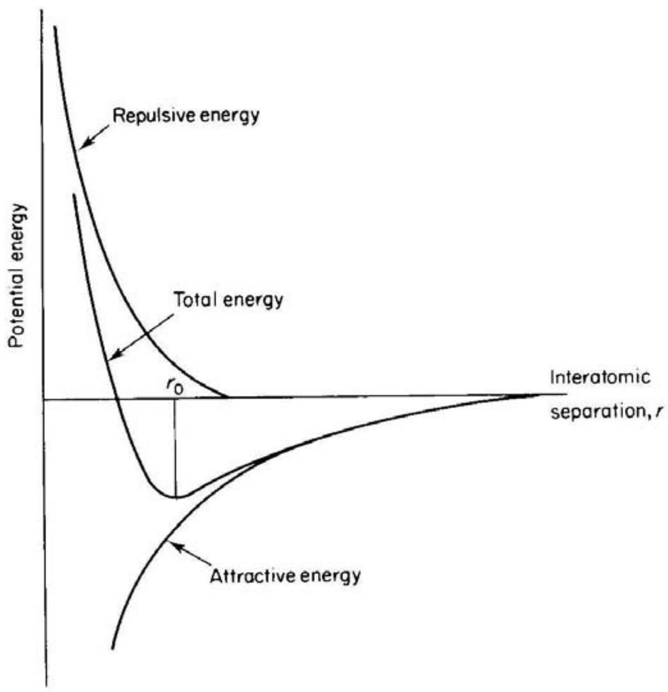
e-content for B.Sc Physics (Honours)
B.Sc Part-III
Paper-VII

Dr. Ayan Mukherjee,
Assistant Professor,
Department of Physics,
Ram Ratan Singh College, Mokama.
Patliputra University, Patna

INTERATOMIC FORCES

It has been shown earlier that the atoms in crystalline solids are arranged in neat ordered structures. Now we will describe the nature of the forces which hold those atoms together.

Consider, first, two identical atoms in their ground states being brought together from an infinite separation.



- Initially, the energy of their interaction is zero.
- As the atoms approach, the ***attractive forces*** increase and the energy increases in a negative sense (the energy of attraction is negative since the atoms do the work, while that of repulsion is positive as work has to be done on the atoms).

- At a separation of a few atomic radii, repulsive forces begin to increase exponentially.
- The atoms reach an equilibrium separation r_0 at which the **repulsive and attractive forces are equal** and **the mutual potential energy is a minimum**.

$$E(r) = -E_{att} + E_{rep}$$

where

$$E_{att} = -\frac{A}{r^n}$$

and

$$E_{rep} = \frac{B}{r^m} \quad \text{or} \quad = B\ \exp\left(\frac{-r}{\rho}\right)$$

Cohesive energy: the energy required to pull the crystal apart into a set of free atoms.

Ionization Energy: Energy required to remove electrons.

Note:

1- Forces which hold solids together are totally electrostatic in origin.

2- Different bonds give rise to different physical properties in solids.

3- Most real bonds are intermediate between the 'extreme' types classified below.

1. THE IONIC BOND

Typical Example: NaCl whose melting point is 801°C

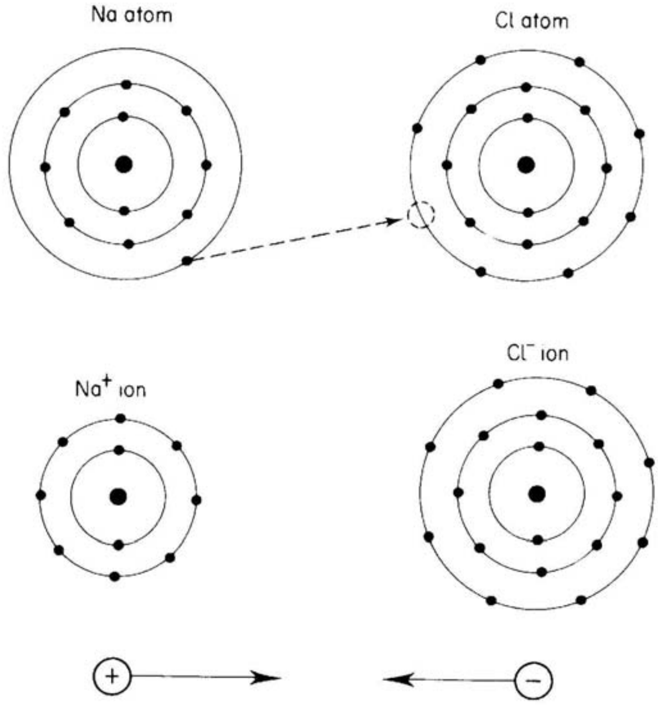
Strength: strong (~5 eV per bond)

Origin:

Transfer of electrons between two atoms

⇒ Formation of (+ve) & (-ve) ions

⇒ Existing of Coulomb force $\dfrac{e^2}{4\pi\varepsilon_0 R^2}$



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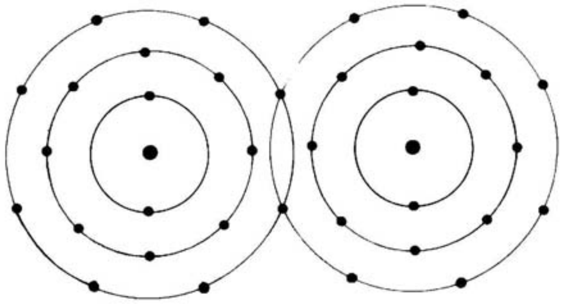
Typical Example: Diamond whose melting point is very high >3000°C

Strength: strong (~few eV per bond)

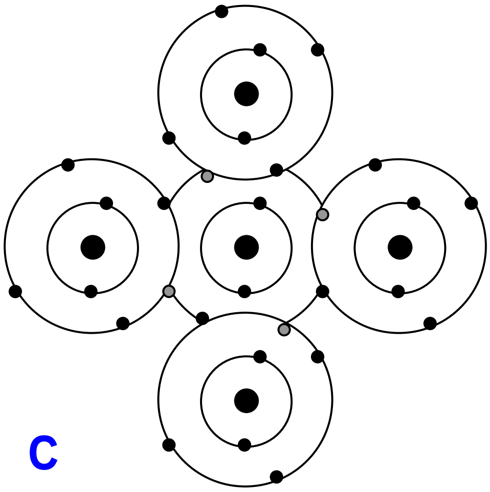
Origin:

Existing of 4 (or2) atoms with 4 (or7) valence electrons ⇒Each atom contributes by one electron

⇒ Formation of a *double-electron* bond



Cl_2



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Type of binding in GaAs:

31% Ionic & 69% Covalent

3. THE METALLIC BOND

Typical Example: Na whose melting point is 97.8^{o}C

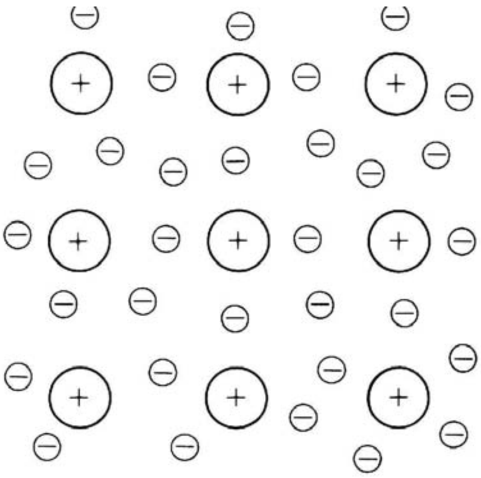
Strength: Somewhat weaker but not negligible

Origin:

Existing of atoms with one or two loosely bound valence electrons

⇒ As atoms become closer, those electrons become free

⇒ Formation of cores of (+ve) ions dispersed in a see of electrons.



4. THE HYDROGEN BOND

Typical Example: Ice (H_2O) whose melting point is just 0°C

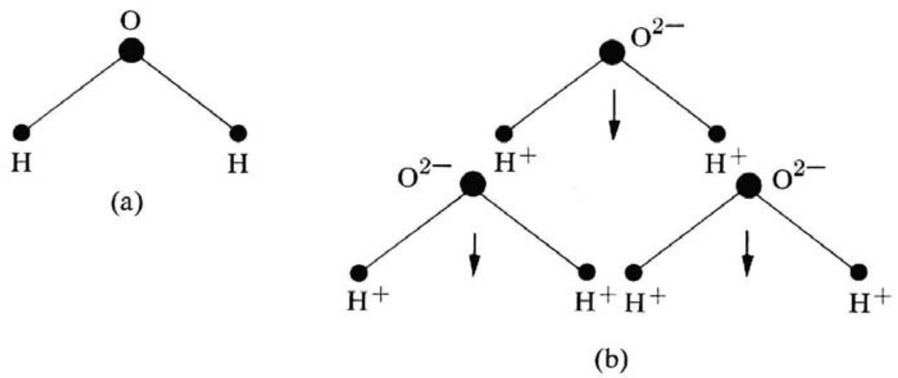
Strength: weak

Origin:

Electrons pulled more strongly toward one atom of a molecule

⇒ Formation of an *electric dipole*

⇒ Molecules which are attracted to each



other

5. VAN DER WAALS BOND

Typical Example: Inert- Gas elements (e.g. He) whose melting point is very low –272.2°C

Strength: very weak

Origin:

Existing of atoms have a completely full outer shell.

⇒ No exchange or sharing of electrons

⟹ Fluctuations of electrons symmetric distribution around the nucleus

⟹ Formation of a fluctuating *electric dipole* on each atom