

CHAPTER 2

INTERATOMIC FORCES

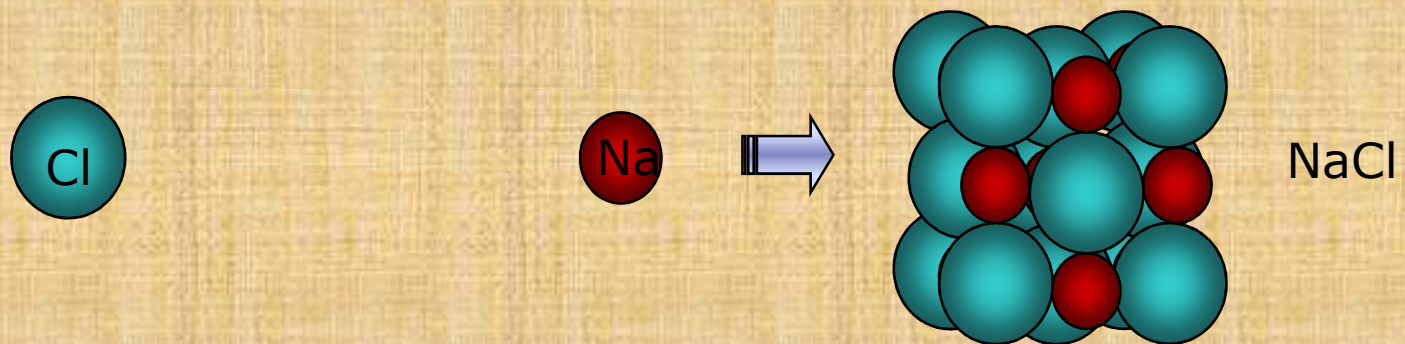
What kind of force holds the atoms together in a solid?

Interatomic Binding

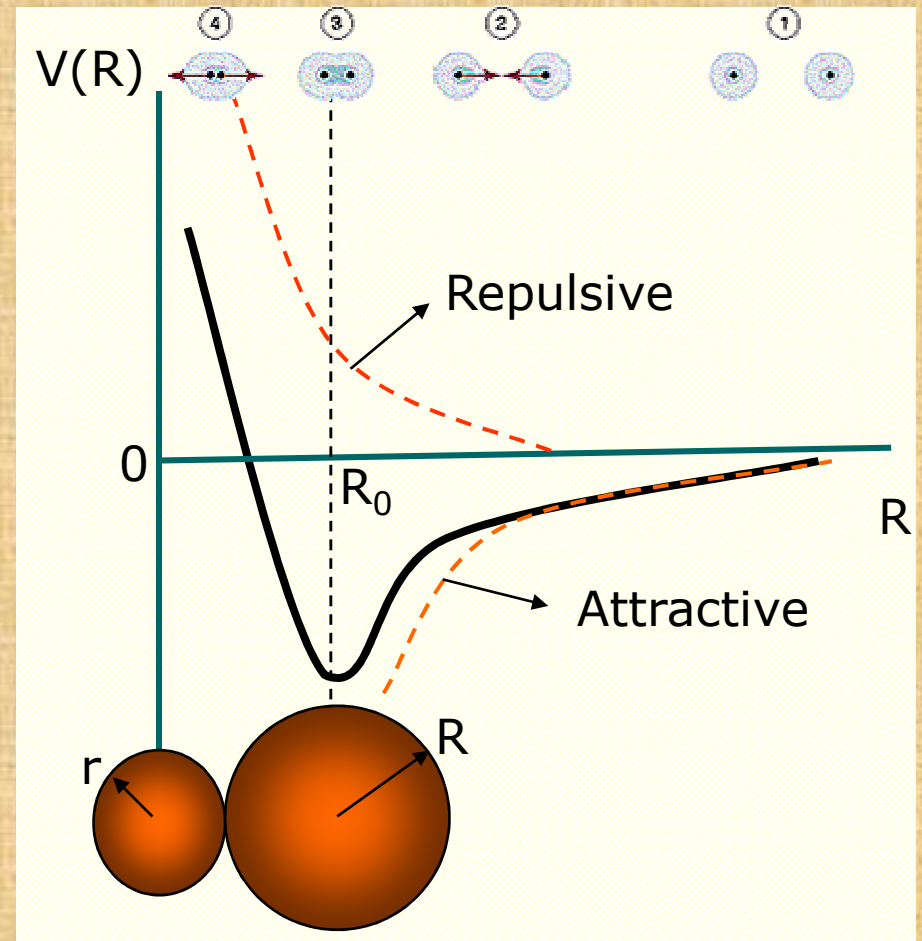
- All of the mechanisms which cause bonding between the atoms derive from electrostatic interaction between nuclei and electrons.
- The differing strengths and differing types of bond are determined by the particular electronic structures of the atoms involved.
- The existence of a stable bonding arrangement implies that the spatial configuration of positive ion cores and outer electrons has less total energy than any other configuration (including infinite separation of the respective atoms).
- The energy deficiency of the configuration compared with isolated atoms is known as cohesive energy, and ranges in value from 0.1 eV/atom for solids which can muster only the weak van der Waals to 7eV/atom or more in some covalent and ionic compounds and some metals.

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.
 - Ge crystal is more stable than a collection of free Ge.



- 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



- Force between the atoms is the negative of the slope of this curve. At equilibrium, repulsive force becomes equals to the attractive part.

The potential energy of either atom will be given by:

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

or simply:

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

V(r): the net potential energy of interaction as function of r

r: the distance between atoms, ions, or molecules

a, b: proportionality constant of attraction and repulsion, respectively

m, n: constant characteristics of each type of bond and type of structure