Energy Bands in Solids

BPT: 401: Electronics and Modern Physics

Tutorial - 1

Electronics

- ❖ The study of electronic devices in which the electrons are transported through a vacuum, gas or semiconductors.
- ❖ The motion of electrons in electronic devices is usually controlled by electric field.
- ❖ Examples of electronic devices are diodes, transistor etc.
- ❖ Electronic devices have wide variety of applications starting from home appliances to medical and space applications.

Electrons

- The electron is one of the fundamental particles constituting the atom. The charge of an electron is negative and is denoted by the symbol e (e = 1.6×10^{-19} coulomb).

- The mass of an electron changes with its velocity in accordance with the theory of relativity. An electron moving with a velocity v has a the mass $m = \frac{m_0}{\sqrt{1 - \frac{V^2}{C^2}}}$ where, c is the velocity of light in free space (c = 3×10^{8} m/s)

  If $v <<< c$, then $m = m_0$ called the rest mass of electron. (m_0 = 9.11×10^{-31} kg)

- An electron from rest and accelerated through a potential difference of 6 kV, acquires a velocity of 0.15c ($1/2mv^2$ = eV). Therefore, the change of mass of an electron with velocity can be neglected for accelerating potential below 6 kV.

- The radius of electron is 10^{-15} m and that of an atom is 10^{-10} m. The radii are so small that electrons and atoms are ordinarily considered as point masses.

Electron volt (unit of energy)

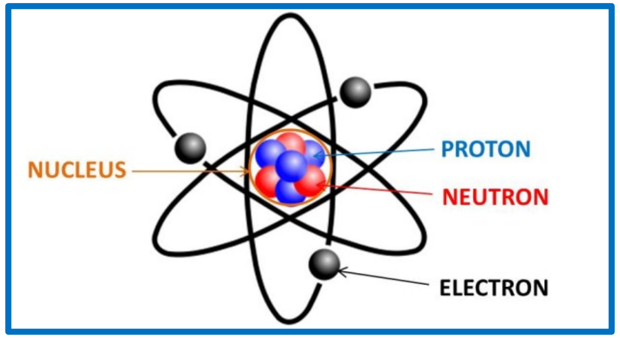
- For energies involved in electronic devices, 'joule' is too large a unit. Such small energies are measured in electron volt (eV).

- The electron volt is the kinetic energy gained by an electron, initially at rest in moving through a potential difference of 1 volt.

- Since e = 1.6×10^{-19} coulomb, 1 electron volt = eV = 1.6 × 10-19 coulomb × 1 volt = 1.6×10^{-19} joule.

Atomic Energy Levels

- An atom of an element is generally made up of electrons, protons and neutrons. The only exception is the hydrogen atom, which possesses one electron and one proton, but no neutron.



- The charge of the proton is numerically equal to that of an electron but proton is positive charge.
- The mass of proton is 1837 times the mass of an electron. The neutron is neutral particle having a mass nearly equal to the proton.
- Since protons and neutrons carry practically the entire mass of the atom, they remain almost immobile in a region called the atomic nucleus.
- The electrons revolve around the nucleus in definite orbits which are circular or elliptical. The atom is electrically neutral because of the number of orbiting electrons equal to the number of protons in the nucleus.

Bohr Atomic Model

Bohr's general assumption:

The electrons are assumed to move about the nucleus in certain discrete circular orbits (like planets orbits the sun).

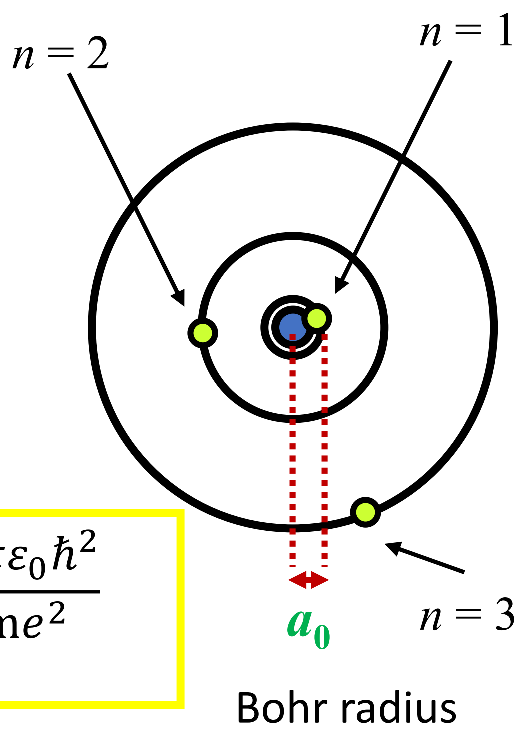
The orbiting electrons do not radiate energy and each discrete orbits have specific energy states. The electron energy is quantized.

Each orbit can hold a specific maximum number of electrons. Electrons fill orbits closest to the nucleus first.

In any orbit, the angular momentum of the electron is equal to an integral multiple of h/2π (where, Plank's constant h = 6.62 × 10^{-34} Js). i.e. $L = n\hbar$

Electrons can make transition between the stationary energy states when $\Delta E = E_1 - E_2 = h\vartheta$ is satisfied.

Classical laws of physics do not apply to transitions between stationary states.



$$a_0 \equiv \frac{4\pi\varepsilon_0\hbar^2}{me^2}$$

Electronic Transitions in atomic energy level: Quantum Mechanical Approach

The wavelengths emitted from the atom due to electronic transitions from higher energy states to lower ones ($E_2 \rightarrow E_1$) give the spectral lines characterizing the atom.

To explain the details of the spectral lines of some elements, four quantum numbers, designated by n, l, m_l *and* m_s have introduced over the Bohr atom model.

The state of an electron in the atom is uniquely specified by the four quantum numbers. According to *Pauli's exclusion principle*, no two electrons in an electronic system can occupy the same quantum state described by the same set of four quantum numbers n, l, m_l *and* m_s

The quantum numbers can take the following values:

- Principal quantum number, $n = 1, 2, 3, \ldots \ldots ..$ [*determines the energy of the orbital electrons*] K, L, M… shells
- Orbital angular momentum quantum number, $l = 0, 1, 2, \ldots, (n-1)$ [*measures the angular momentum of e*$^-$]

  s, p, d ,f …. subshells
- Magnetic quantum number, $m_l = 0, \pm 1, \pm 2, \ldots \ldots \pm l$ [*gives splitting of energies for a given* n *and* l *in a magnetic field*]
- Spin quantum number, $m_s = \pm \frac{1}{2}$ [*shows spin of electron about its own axis is quantized*]

$For\ n = 1\ (K\ shell)$

$\rightarrow l = 0\ (s\ subshell), ml = 0\ \&\ m_s = \pm 1/2$

There are two states for n=1, the two states ($m_s = +1/2\ \&- 1/2$) are called 1s states

2 electron states

$For\ n = 2\ (L\ shell)$

$\rightarrow l = 0\ (s\ subshell), ml = 0\ \&\ m_s = \pm 1/2$ two 2s states

$\rightarrow l = 1\ (p\ subshell), ml = -1, 0, 1\ \&\ m_s = \pm 1/2$ six 2p states

8 electron states

$For\ n = 3\ (M\ shell)$

$\rightarrow l = 0\ (s\ subshell), ml = 0\ \ \&\ m_s = \pm 1/2$ two 3s states

$\rightarrow l = 1\ (p\ subshell), ml = -1, 0, 1\ \ \&\ m_s = \pm 1/2$ six 3p states

$\rightarrow l = 2\ (d\ subshell), ml = -2, -1, 0, 1, 2\ \ \&\ m_s = \pm 1/2$ ten 3d states

18 electron states

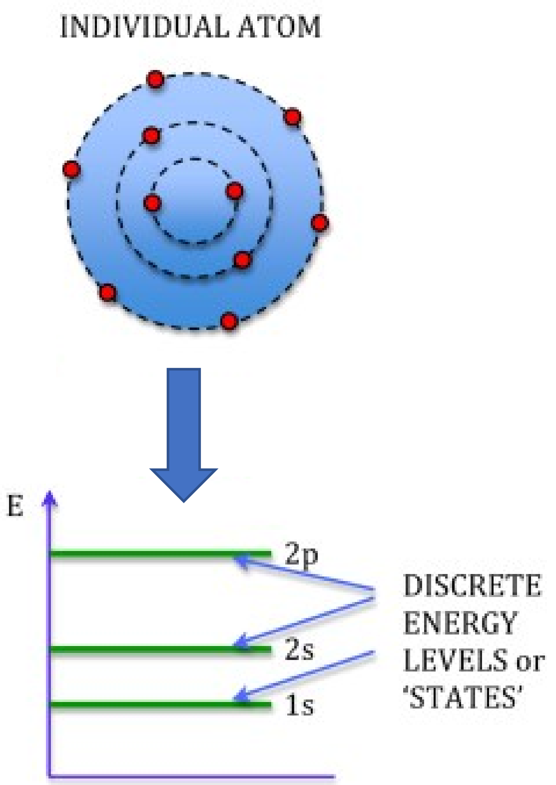
Obeys Pauli's exclusion Principle

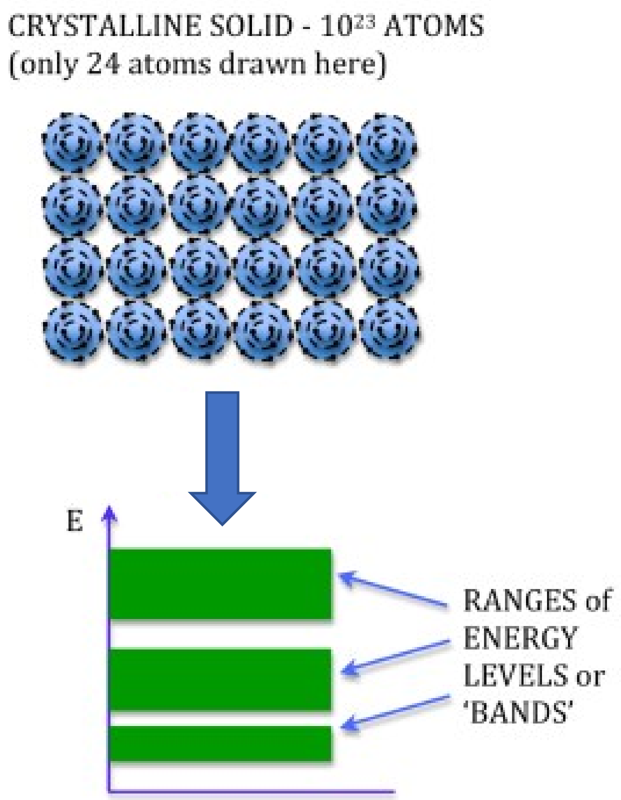
Energy Bands in Crystals

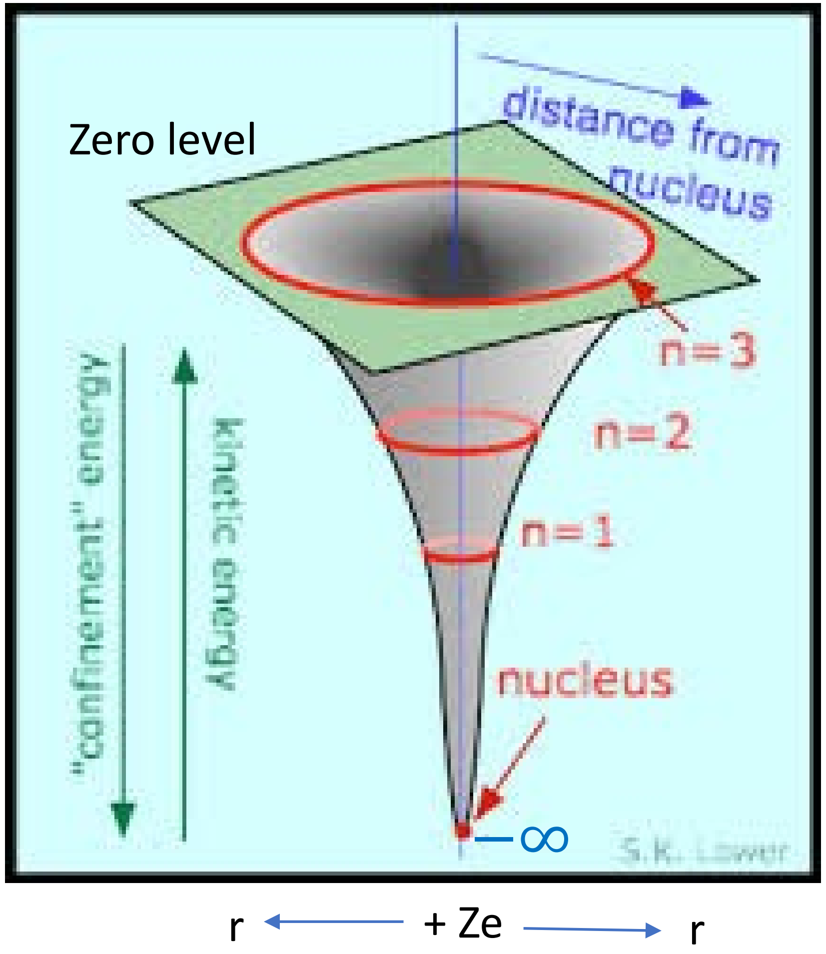
The potential energy of electron of charge -e at a distance r from the nucleus of charge +Ze is $E_p(r) = -Ze^2/4\pi\varepsilon_0 r^2$

Total energy of an electron in an atom is kinetic plus potential energy, is negative and has discrete values.

A crystal is a solid consisting of a regular and repetitive arrangement of atoms or ions in 3-dimension space.







Potential energy of electron with its distance from the nucleus

Energy Bands in Crystals

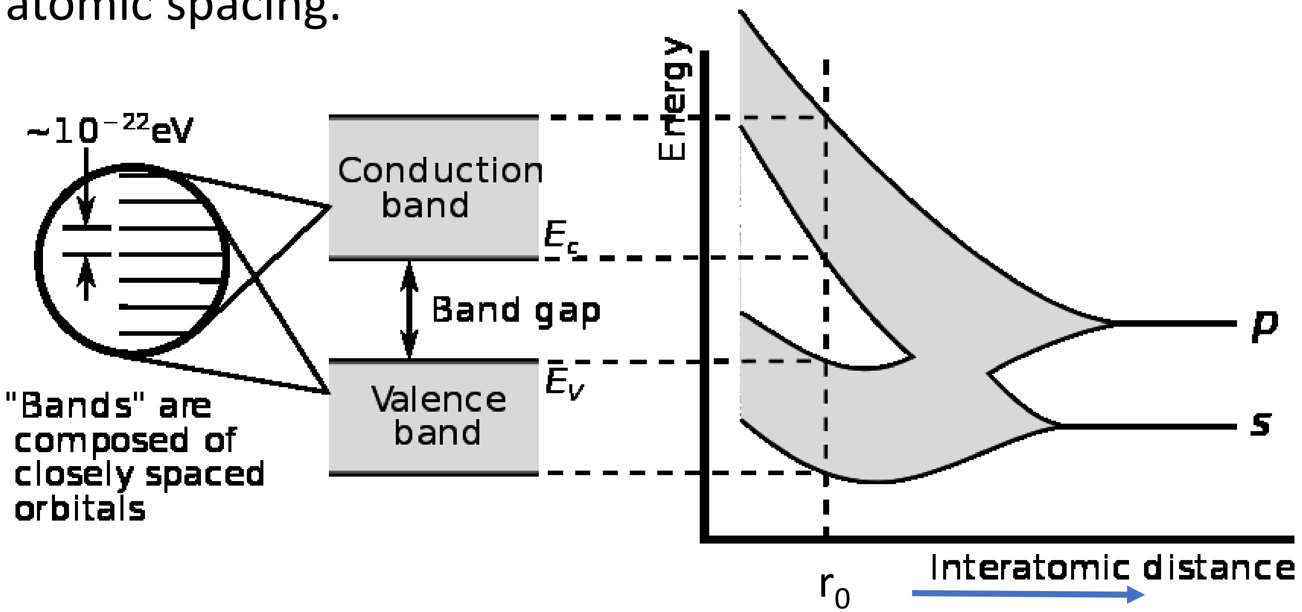
When a number of atoms are brought close together to form a crystal, the discrete energy levels of individual atoms overlap due to interatomic coupling and forms an energy bands composed of closely spaced orbitals, so that Pauli's exclusion principle is satisfied.

The lower energy levels are not greatly affected by the interaction among neighboring atoms, and hence form narrow bands. The higher energy levels are greatly affected by the interatomic interactions and produce wide bands.

The interatomic spacing is fixed and different for different crystals and the width of energy band depends on the type of crystal. It is larger for a crystal with smaller interatomic spacing.

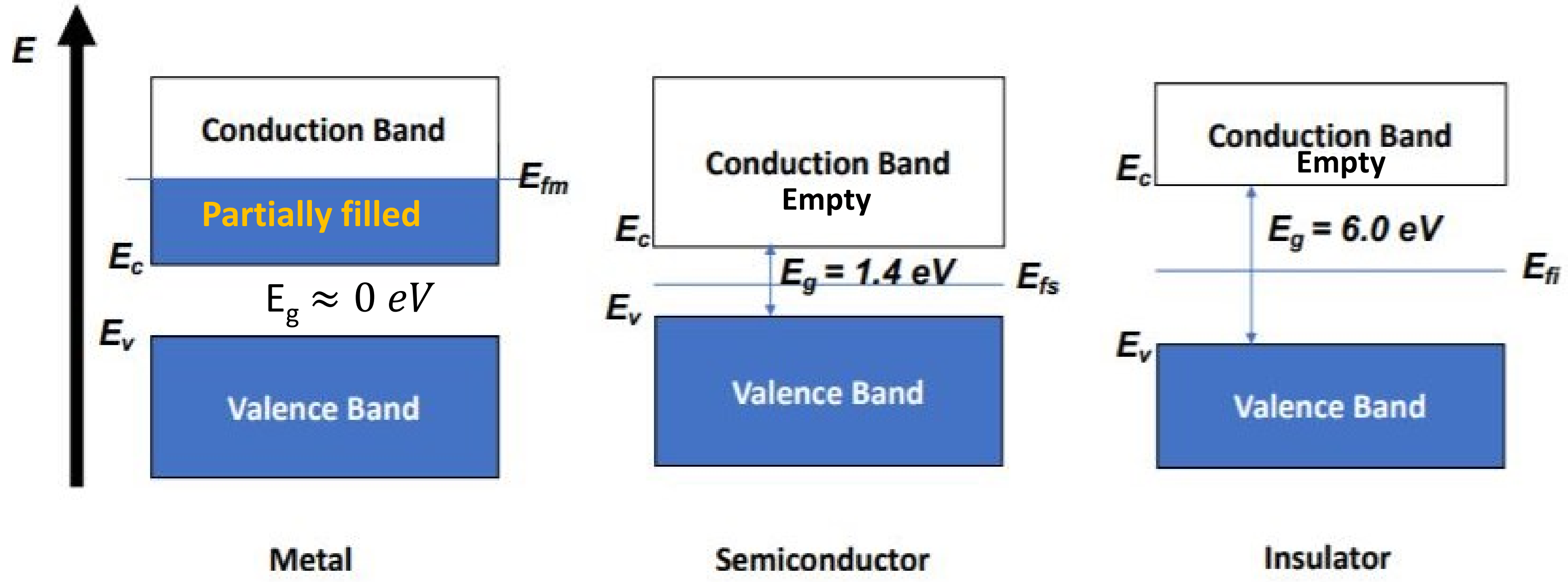
The width of band is independent of the number of atoms in the crystal but the number of energy levels in a band is equal to the number of atoms in the crystal

Lower energy levels are completely filled by the electrons and higher energy levels may be completely empty or partially filled by electrons.



As the allowed energy levels of a individual atoms expands into energy bands in crystal, the electrons in a crystal can not have energies in the region between two successive bands. This energy gap is called forbidden gap or band gap.

Metal , Insulator and Semiconductor



Metal

- Partially filled Conduction Band
- E_V and E_c overlap ($E_g \approx 0\ eV$)
- Fermi energy in Conduction Band
- Free electrons in Conduction Band

Semiconductor

- Empty Conduction Band
- Small energy gap between E_V and E_c (E_g between 0.3 to $3\ eV$)
- Fermi energy in the middle of E_g
- At 0 K, no free electrons in Conduction Band
- Free electrons in Conduction Band increases with temperature

Insulator

- Empty Conduction Band
- Large energy gap between E_V and E_c ($E_g \gg 3\ eV$)
- Fermi energy in the middle of E_g