PYL102 Course
Lecture-7 on 23-08-2021

Course coordinator: Rajendra S. Dhaka (Rajen)

(rsdhaka@physics.iitd.ac.in) http://web.iitd.ac.in/~rsdhaka/

PYL102:
Principles of Electronic Materials

- Summary of K-P model outcome……
- Formation of energy band…
- Energy bands in solids ……..
- Understanding metal, semiconductor and insulator….

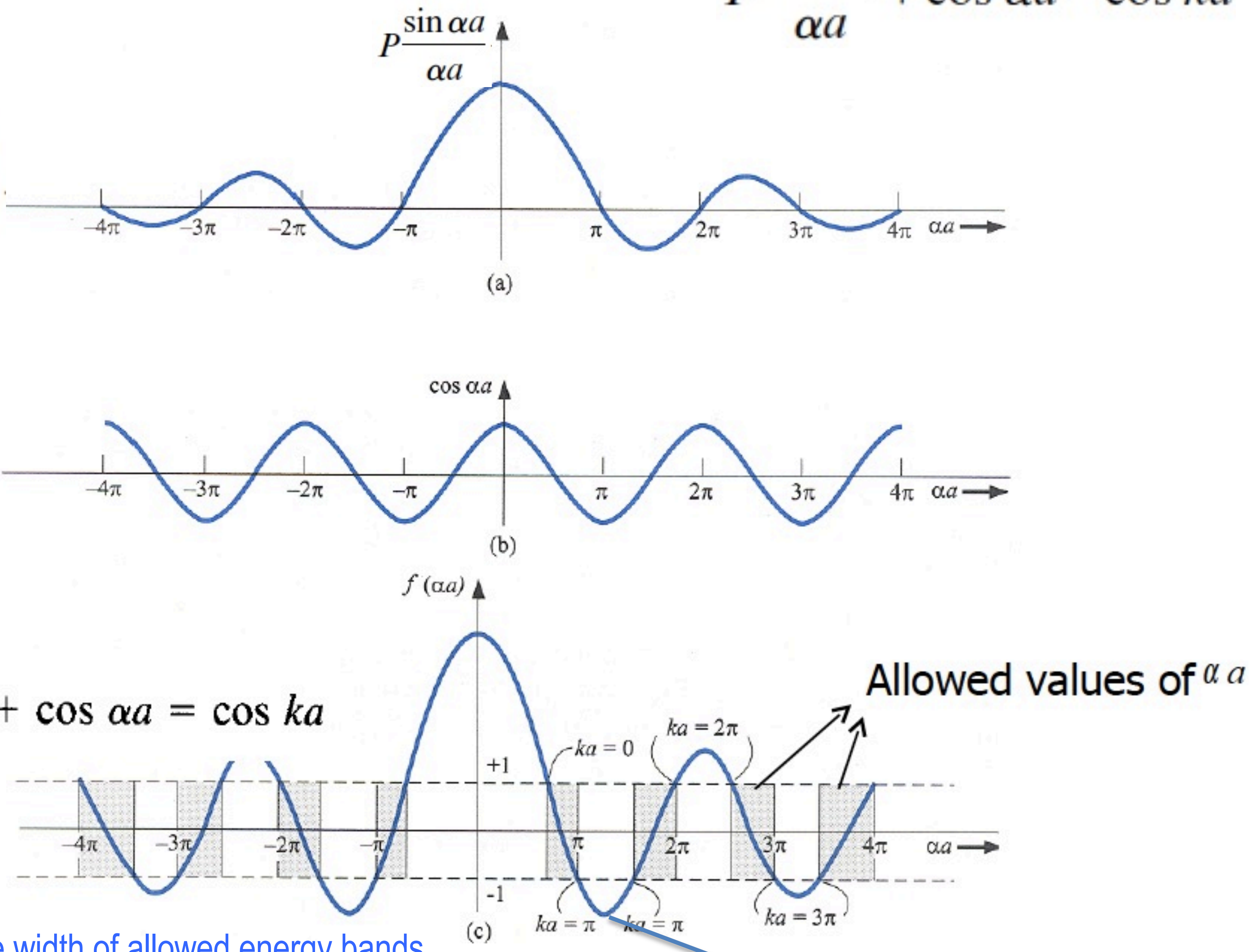
Energy band formation

$$P\frac{\sin \alpha a}{\alpha a} + \cos \alpha a = \cos ka$$

$$P\frac{\sin \alpha a}{\alpha a}$$

$$\cos \alpha a$$

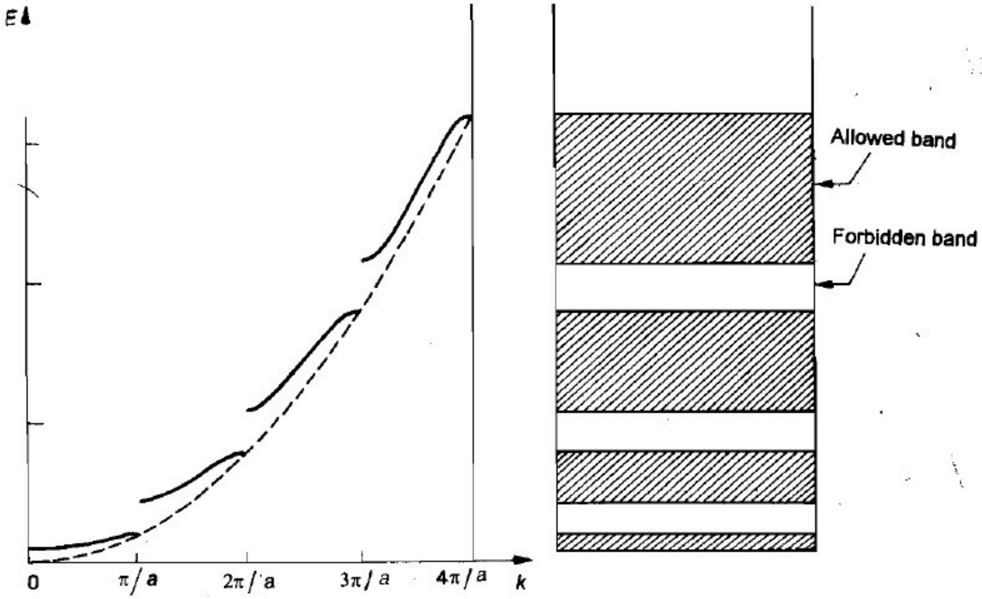
$$P\frac{\sin \alpha a}{\alpha a} + \cos \alpha a = \cos ka$$



Q: show that the width of allowed energy bands increases as energy of electron is increased.

Energy band formation

✧ The dispersion relation can be numerically calculated, and the results are shown below: allowed energy bands….



Interestingly, the E-k relation deviates from the free e^- parabola ($E = \hbar^2k^2/2m$) and an energy discontinuity appears at every $k = n\pi/a$ ($n = \pm1, \pm2, \ldots$.)

i.e. there exist energy ranges which electrons are not allowed to occupy.

Each of these energy ranges is called a forbidden energy band.

❖ Notice that forbidden energy band appears as a result of the interaction of the conduction electron with the periodic lattice potential,….. this is considered in Bloch theorem…..

❖ Ionic potential cause a gap to appear in the E-k plot whenever k crosses a Bragg plane.

❖ Since the BZs are formed by the intersection of Bragg planes, gaps in E-k open as k crosses the boundary of any BZ.

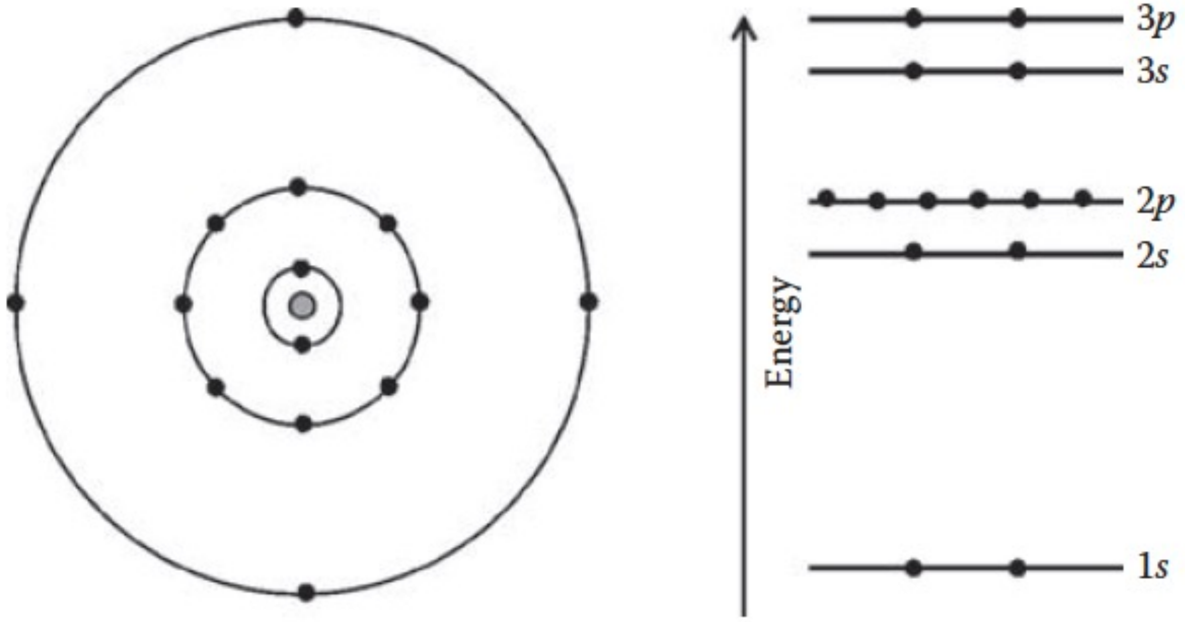
❖ The discontinuities in E-k curve occur at $k = n\pi/a$, These k values define the boundaries of the 1st, 2nd etc. BZs, Within a given energy band, the energy is a periodic function of k..

Origin of band formation in solids:

Tight-binding model:

Diagrams of electron shells (orbits) surrounding a nucleus are a common sight when learning about atomic physics. However, in solid state physics it is more usual to depict these shells as straight lines.

Each electron shell has a different value of energy, as does each corresponding line—which is known as an energy level.



The tight-binding model reveals what happens when a very large number of atoms an infinite distance apart come closer together to form a solid. As the atoms approach one another to form the solid, the wave functions of their electrons start to overlap….

Origin of band formation in solids:

The interactions between the electrons cause the discrete energy levels of each of the isolated atoms to split into a huge number of energy levels forming a band of levels.

This prevents the Pauli exclusion principle from being violated, as while two atoms can have their electrons in exactly the same levels as one another if they are isolated, this cannot occur with the atoms side by side in a solid.

If it did, this would mean electrons with exactly the same set of quantum numbers would be in the same energy level, which is not allowed by the Pauli principle.

So, the split levels created when a solid is formed get round this problem by providing enough separate states to accommodate all the electrons in the solid with the same quantum numbers.

These energy levels are in fact so close together within the bands that they can be considered to be a continuum of levels rather than a collection of discrete energy levels.

When atoms are brought together and band to form a hypothetical solid of atomic number density ~10^{22-23} cm^{-3}.

We do not get 10^{22-23} cm^{-3} identical ground state energy levels, instead, 10^{22-23} cm^{-3} identical levels for the atoms when they are isolated turns into 10^{22-23} cm^{-3} closely spaced energy levels in a band when they are in the solid.

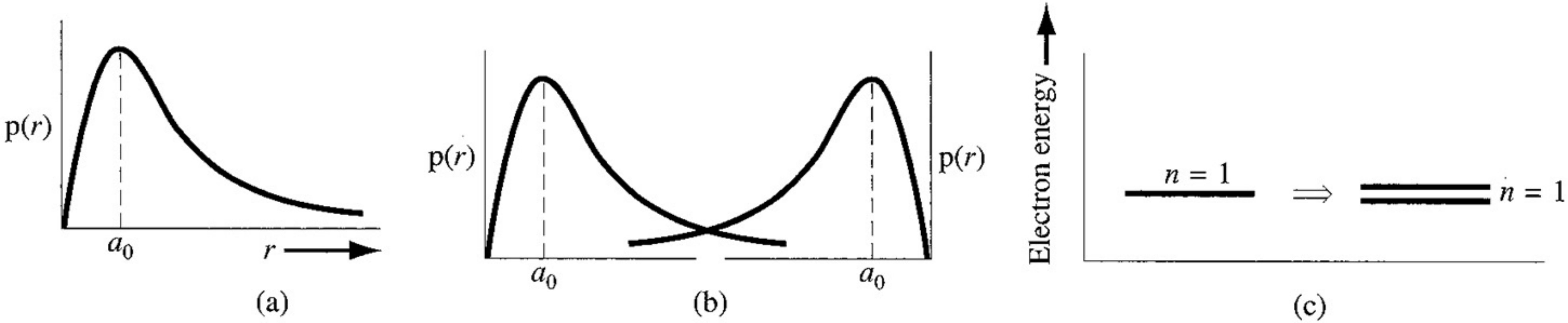
This idea is just an extension of the situation that occurs when two atoms come together to form a molecule. Taking hydrogen as a simple example,…see next slide….

Origin of band formation in solids:

In case of a single isolated atom, there are single energy levels. But when two identical atoms are brought closer the outer most orbits of these atoms overlap and interact.

When the wave function of the electrons of the two different atoms begin to overlap considerably. The energy levels corresponding to those wave functions split into two.

When two hydrogen atoms are brought close enough for the wave functions of n=1 electrons to start interacting, the n=1 state splits into two different energies, in accordance with Pauli exclusion principle.



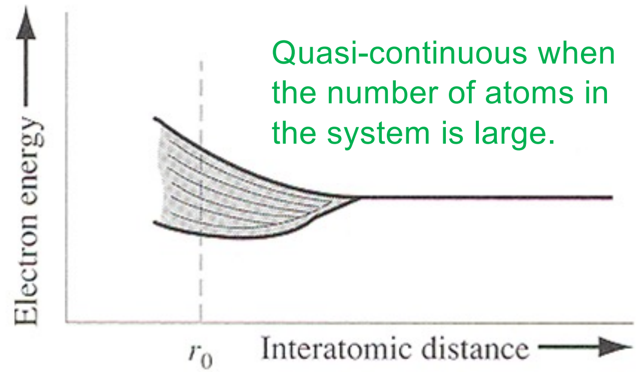
(a) Probability density function of n=1 electron in an isolated hydrogen atom.
(b) Overlapping probability density functions in two adjacent hydrogen atoms.
(c) splitting of n=1 state.

If more atoms are brought together, more levels are formed and for a solid of “N‟ atoms. Each of the energy levels of an atom splits into N levels of energy. The levels are so close together that they form an almost continuous band.

Origin of band formation in solids:

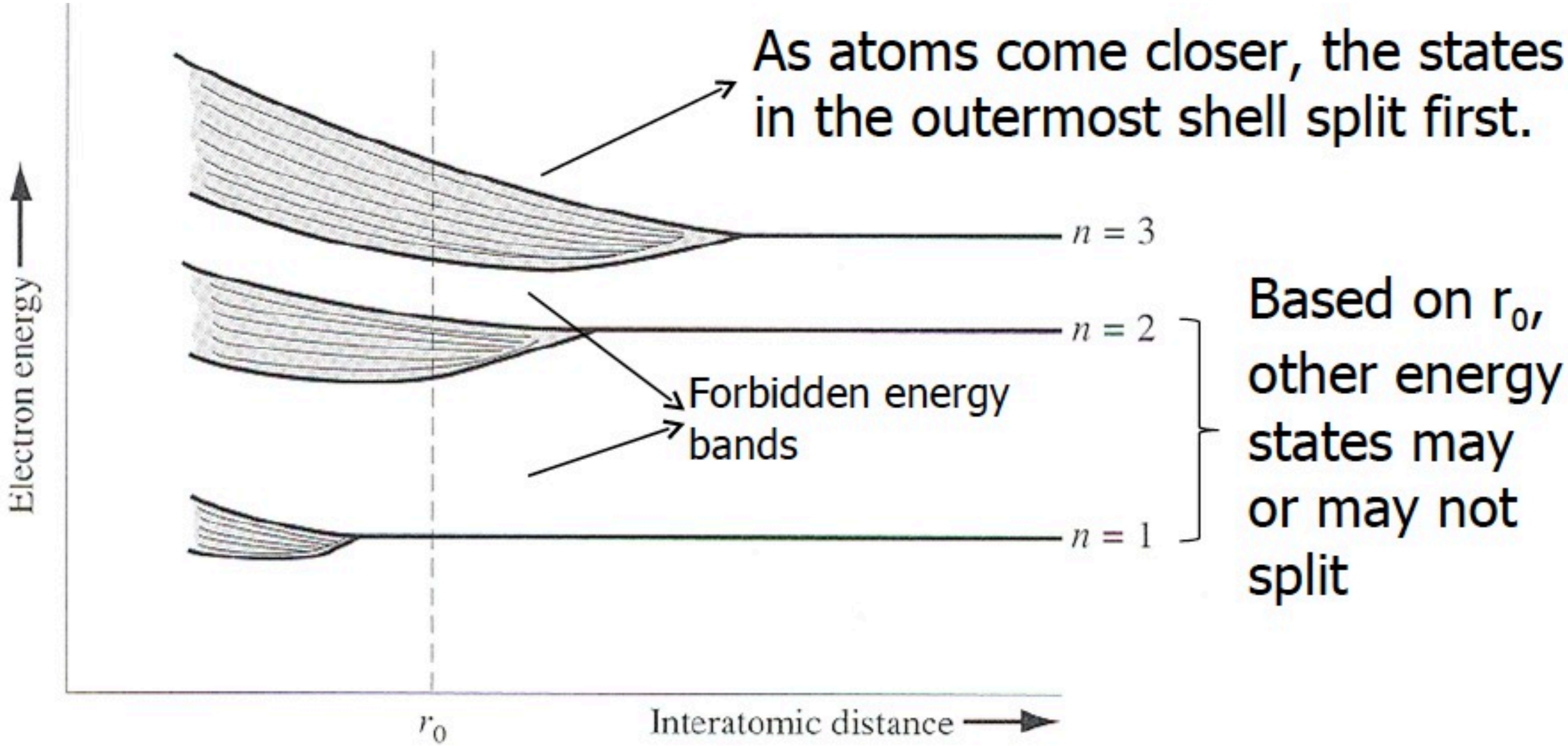
Hypothetically, if we have a periodic arrangement of many hydrogen atoms and they are brought close enough → initial quantized energy level will split into band of discrete levels…

The splitting of an energy state into a band of allowed energies (r_0 is the equilibrium inter-atomic distance in the crystal)



What happens in an atom containing many more electrons?

Splitting of energy states into allowed bands of energies in an atom containing electrons up to n=3.



PYL102 Course
Lecture-8 on 25-08-2021

Course coordinator: Rajendra S. Dhaka (Rajen)

(rsdhaka@physics.iitd.ac.in) http://web.iitd.ac.in/~rsdhaka/

PYL102:
Principles of Electronic Materials

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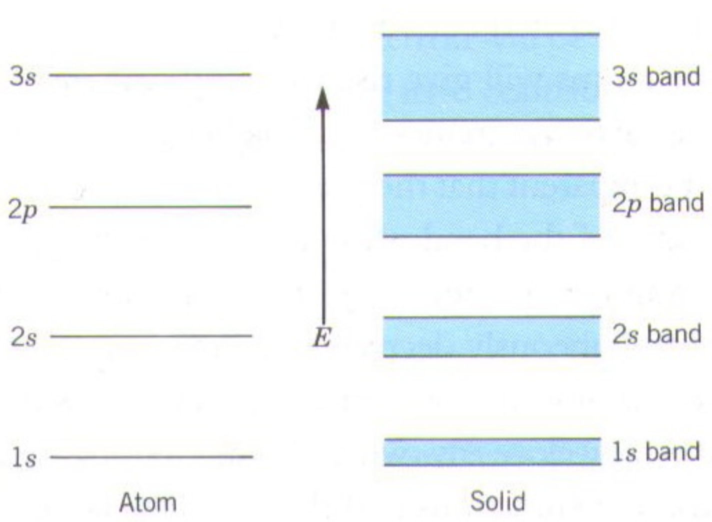
- Energy bands in solids….. …
- Classification of electronic materials……
- Understanding metal, semiconductor and insulator….

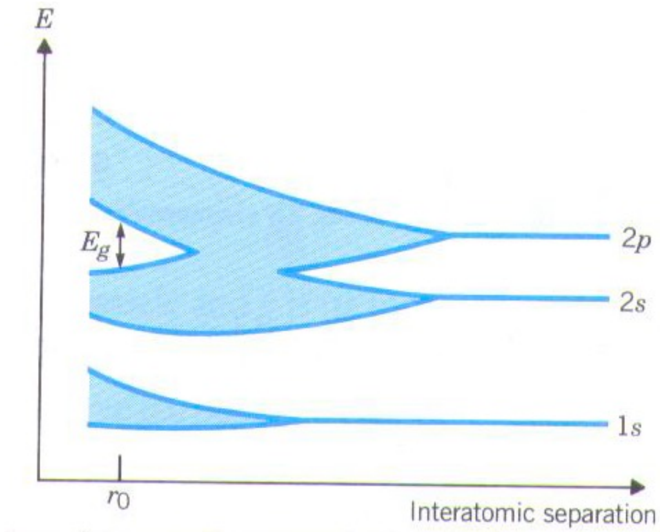
Origin of band formation in solids:

The wave functions of the outermost electron shells that overlap more than those of the electrons closest to the nucleus.

The width of this band depends on the degree of overlap of electrons of adjacent atoms and is largest for the outermost atomic electrons.

Hence, in case of a solid instead of single energy levels associated with the single atom, there will be bands of energy levels for the entire solid…





In fact the outermost electrons can take part in conduction because the overlap of the outermost e^- wave functions is so great it actually extends throughout the whole solid.

The electrons nearest to the nucleus remain bound to the nucleus…in fact only a small number actually take part in conduction….

Band theory of solids:

We know that electrons can have any of the values of energy contained within the energy bands. This means they can move about within the energy bands as moving means changing their kinetic energy, which in turn means changing their energy level, and in a band, there are empty levels nearby that electrons can move into.

This is important to explains the difference between conductors, insulators, and semiconductors, as each different type of solid has a different band structure…..

We can define the top fully filled (at least at T = 0 K) band as the **Valence Band** (VB)…

The next higher energy band is the **Conduction Band** (CB), this band can be empty or partially filed….

The energy difference between the bottom of the CB and the top of the VB is called the **Band Gap** (or forbidden gap)….

In some cases, when sufficient energy is supplied electrons jump from the VB to the CB by overcoming the band gap and thus resulting in the flow of current

As we have seen in previous classes, the Fermi distribution function and how it changes with the temperature…

Note that only those electrons in the materials that are close to Fermi level participate in the conduction of electricity and heat….

Band theory of solids:

- This is because electrons just below the Fermi level gain enough thermal energy to occupy the states that are available….
- For a small thermal energy window, the electrons that are far below the Fermi level can not be excited as they do no have vacant energy states to occupy. Therefore, they normally do not participate in the conduction.
- Electrical conduction will occur if the highest occupied energy band is partially filled.
- We can classify the materials based on the type of band structure they posses (which determines the availability of free electrons and henceforth behavior of conductivity) into conductors, semiconductors, and insulators….
- This distinction is widely used because not only do metals, semiconductors, and insulators have different electrical and thermal characteristics, they also have different optical properties—some of which are exploited in important devices like solar cells, light-emitting diodes, etc.
- Plotting the available energies for electrons in the materials provides a useful way to visualize the underlying difference in these materials…
- In metals, the highest energy band is partially filled and there are higher energy states within the band available for the electrons to go to if their energies are somewhat increased by an externally applied electric field or temperature…

Metals, insulators, and semiconductors:

- Overlap between the occupied and unoccupied band allows the electrons to freely drift between the bands. That means the outer electrons require a very little or no energy to move to other energy states. Applied electric field provides sufficient energy for electrons to occupy empty states. (free electrons)→ case of metals
- However, it is very important to note that the band overlapping is not always the case irrespective of how many number of levels are lying in a proximity.
- We have seen the occurrence forbidden energy regions mathematically in KP model
- In some materials there still exists a gap between the highest occupied energy levels and empty bands. (band gap)→ case of insulators and semiconductors
- In insulators, all the energy bands are completely full of electrons. So, in this case the first empty band is separated by a forbidden energy gap from the highest filled band as we discussed in the energy band scheme of solids……
- These electrons are, therefore, unable to move in the entire solid and they are consequently unable to carry electric current.
- The separation in energy between the top of the VB and the bottom of the next empty band (CB) is the energy gap and is generally denoted by the symbol E_g.
- In an insulator E_g is very large and it is unlikely that electrons in the VB will be able to make it to the CB and, hence, the material remains always insulating….

PYL102 Course
Lecture-9 on 26-08-2021

Course coordinator: Rajendra S. Dhaka (Rajen)

(rsdhaka@physics.iitd.ac.in) http://web.iitd.ac.in/~rsdhaka/

PYL102:
Principles of Electronic Materials

- Formation of energy bands………
- Energy bands in solids….. …
- Classification of electronic materials……
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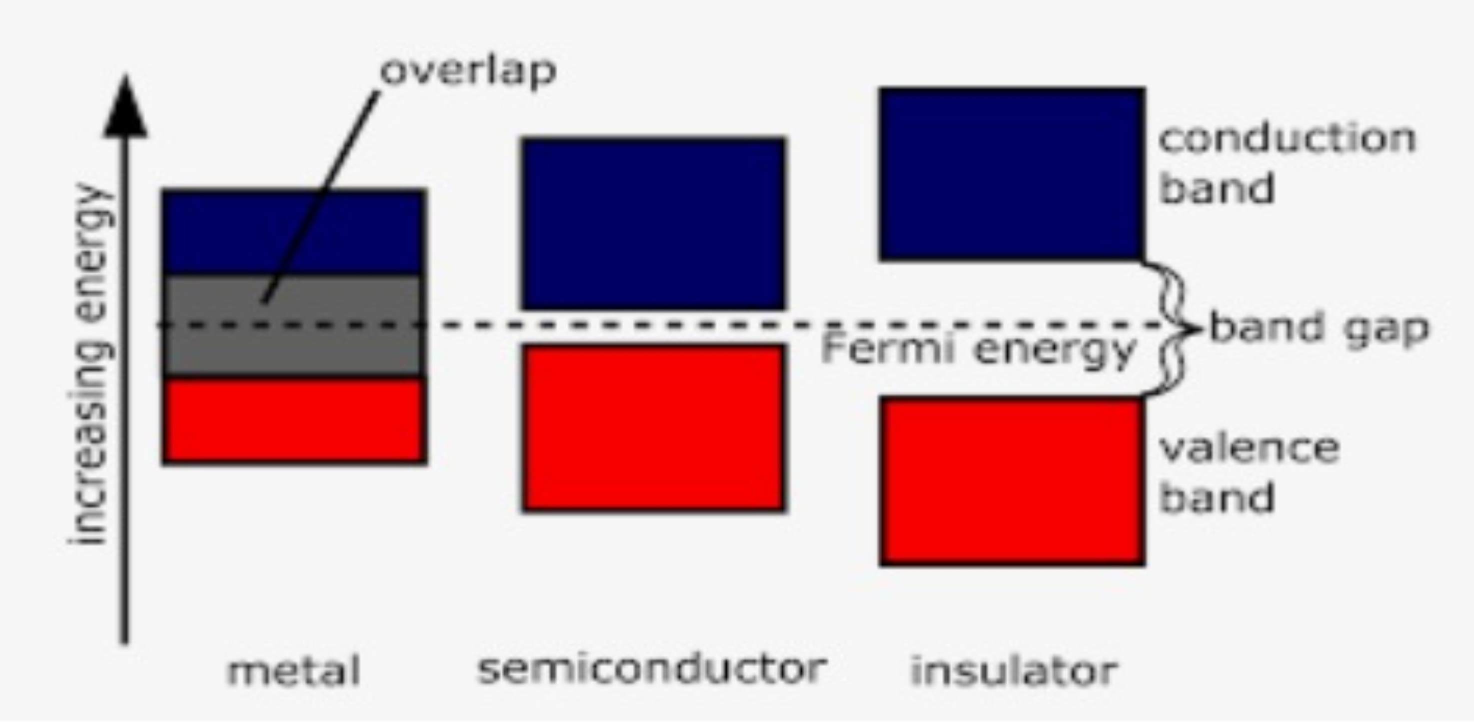
Metals, insulators, and semiconductors:

❖ The band scheme of a semiconductor is essentially similar to that of the insulator ; the highest band is completely full of electrons…

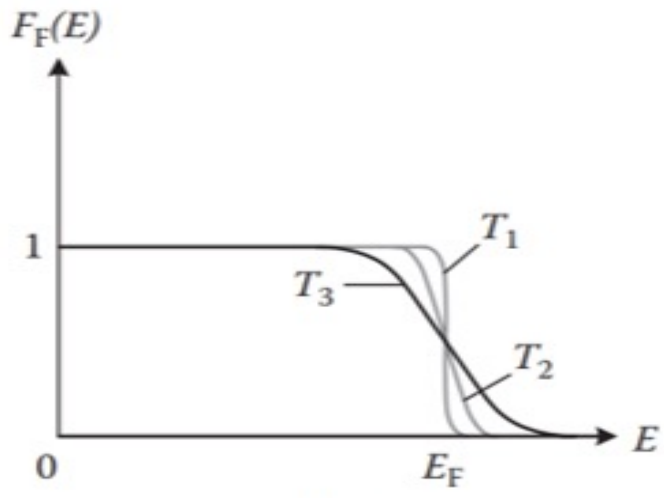
❖ However, in a semiconductor the energy gap E_g is small and electrons in the VB can potentially acquire enough energy to surmount this energy gap and make it to the conduction band. These electrons will, therefore, become free and available for conduction in the presence of an electric field across the semiconductor.

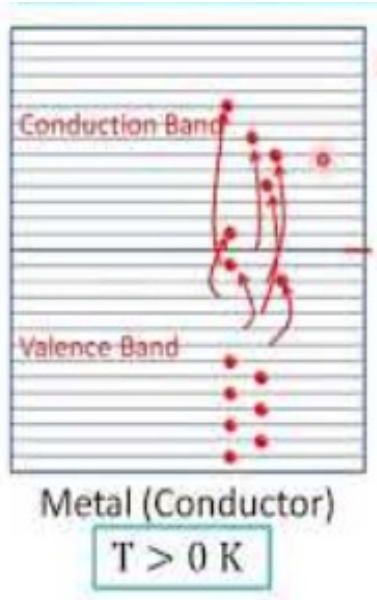
❖ Generally, in a semiconductor this energy E_g required to raise the electron to the conduction band can be supplied as thermal energy.

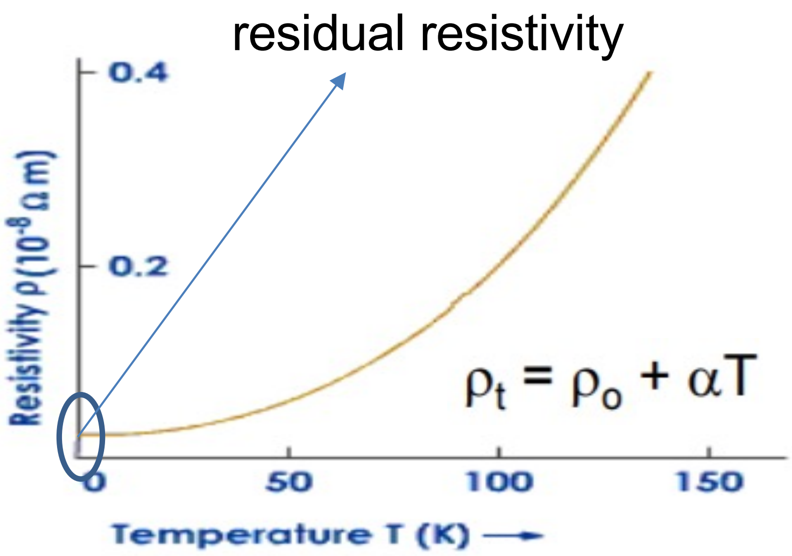


Metals:

As the levels are closely spaced to each other in energy and there is an overlap between the bands, generally the energy provided by the electric field or temperature is sufficient to stimulate an electrons to any empty states







- Resistivity typically increases linearly with temperature, where ρ_o and α are constants for a specific material….
- The number of electrons in the CB does not vary with temperature.
- But increase in temperature increases the scattering events.

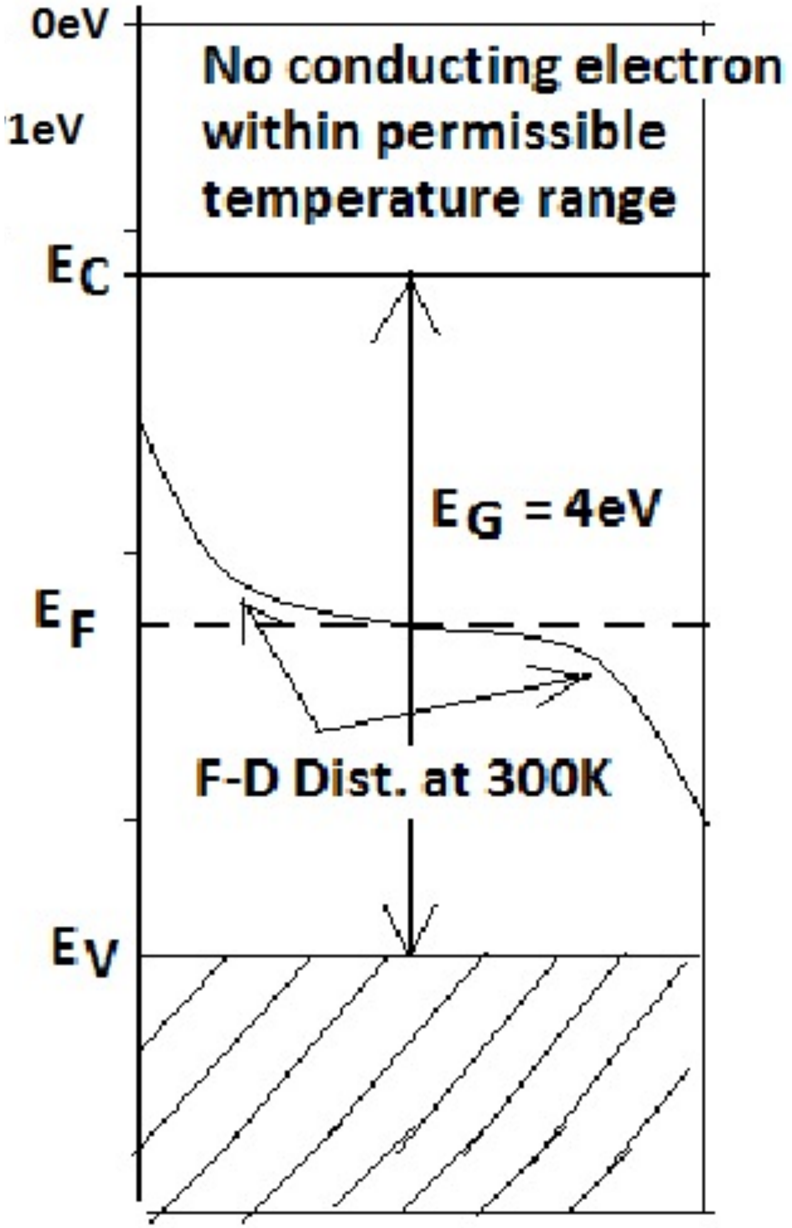
Insulators:

- Insulators are the materials which don't allow the flow of electrons through them!!
- Insulators possess a high resistivity and low conductivity.
- Their atoms have tightly bound electrons that do not move throughout the material. Because the electrons are static and not freely roaming, the current cannot pass through easily.

- High resistance, breakdown voltage and air permeability are the basic properties of insulators ..
- The valence band and conduction band are separated by a large (> 4eV) energy gap, which is a "forbidden" range of energies.

- Electrons must be promoted across the energy gap to conduct, but the energy gap is large, here.
- Diamond is an insulator with a band gap of about 6eV!!!!!

Insulators:



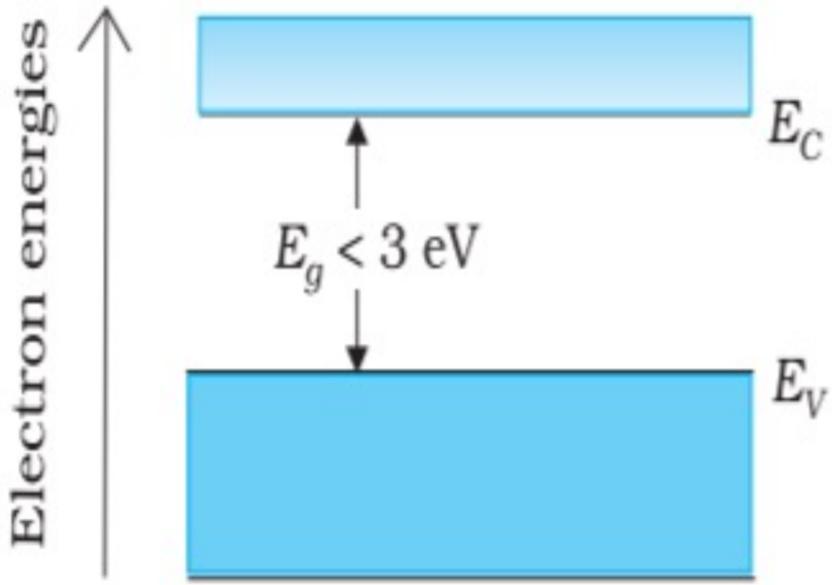
- At T = 0, lower valence band is filled with electrons and upper conduction band is empty, leading to zero conductivity.

- Fermi level E_F is at midpoint of large energy gap (2-10 eV) between conduction and valence bands.

- At T > 0, electrons are usually NOT thermally "excited" from valence to conduction band, leading to zero conductivity

Semiconductors:

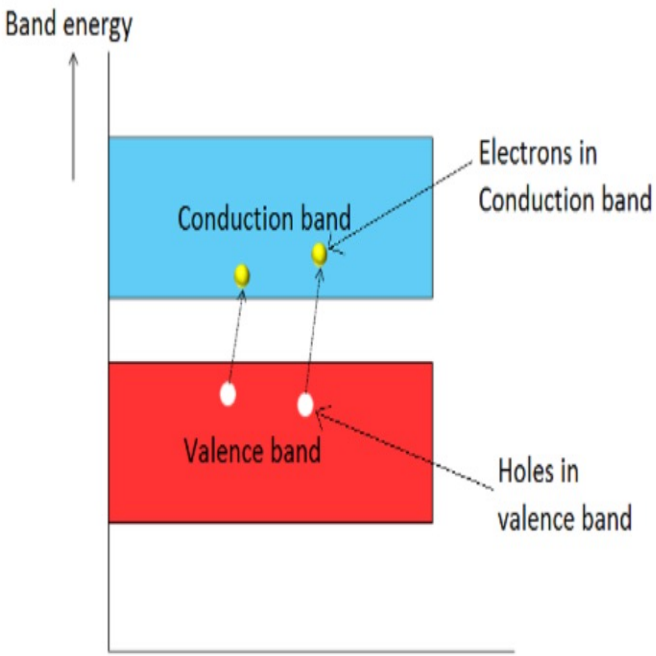
Band scheme for intrinsic conductivity in a semiconductor



A finite but small band gap (Eg < 3 eV) exists

At 0 K the conductivity is zero because all states in the VB are filled and all states in the CB are vacant

As the temperature is increased, there is a finite probability that an electron is thermally excited from the VB to the CB, where they become mobile. Such carriers are called “**intrinsic**.”



When an electron is excited to CB from a VB it leaves behind an unoccupied state known as hole.

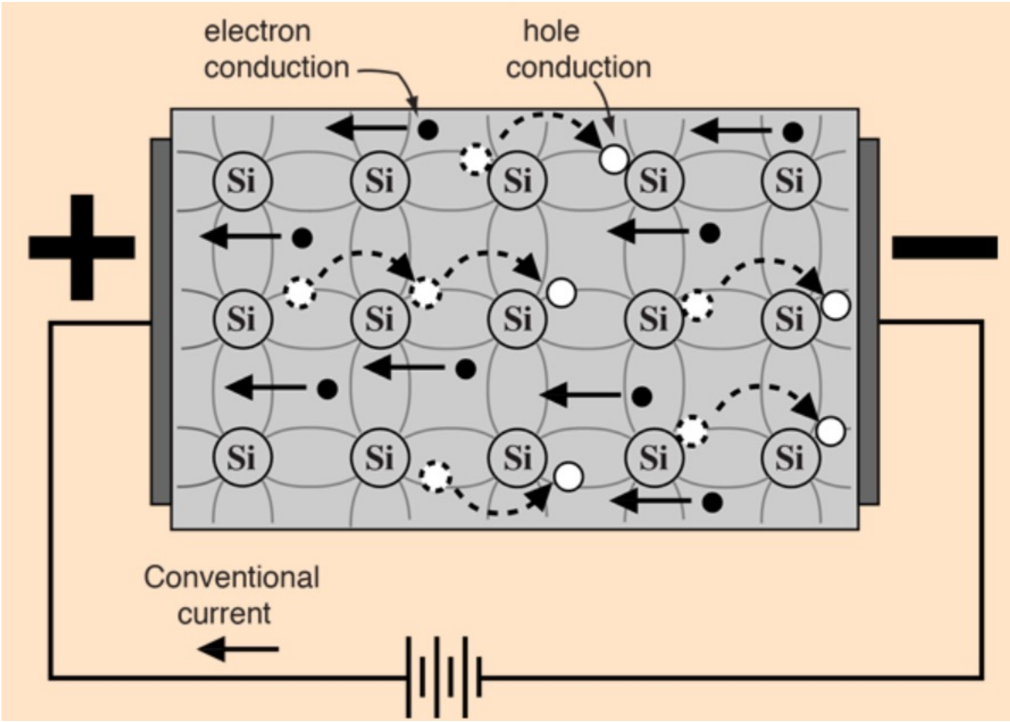
Holes are therefore absence/deficiency of an electron…

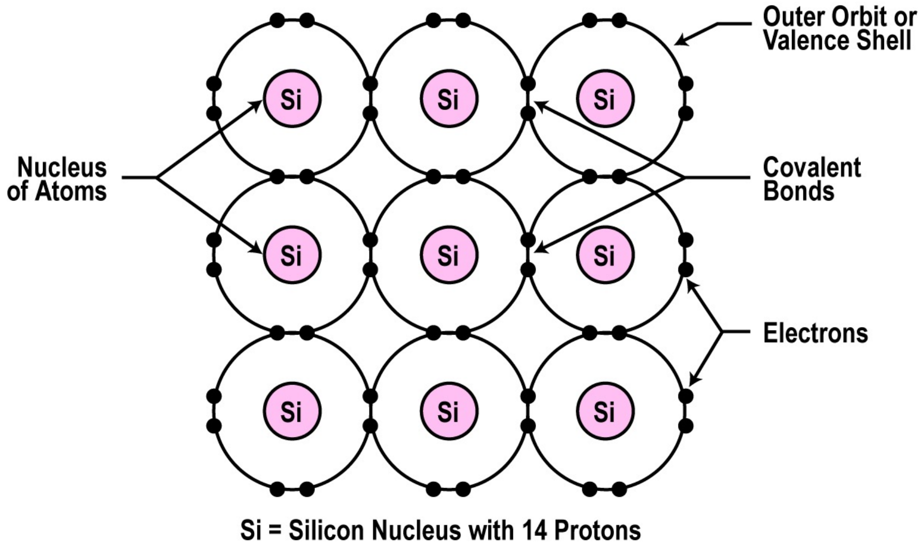
Hole is a positively charged carrier and has a charge equal to that of an electron but with an opposite polarity

Holes also participate in total conduction.

Holes in a semiconductor can move in crystal lattice like electrons and play an important role in conduction.

Semiconductors:





- The total current in the semiconductor on the application of voltage will be consisting of contributions from both the holes and electrons.

- Movement of the holes will be due to the jumping of neighboring electrons into the holes. Holes will move in opposite directions to the electrons and contribute positively to the current as they posses a positive charge.

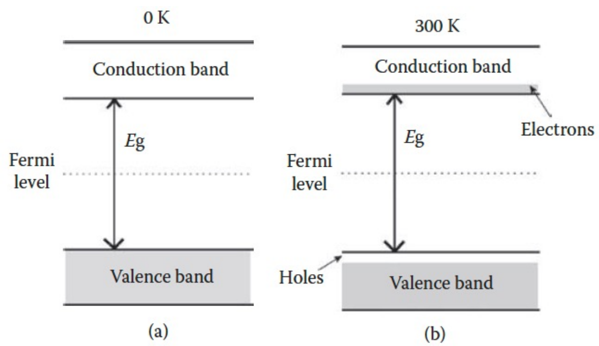
- Holes have effective mass higher compared to their electron counterparts meaning that they are less mobile compared to electrons.

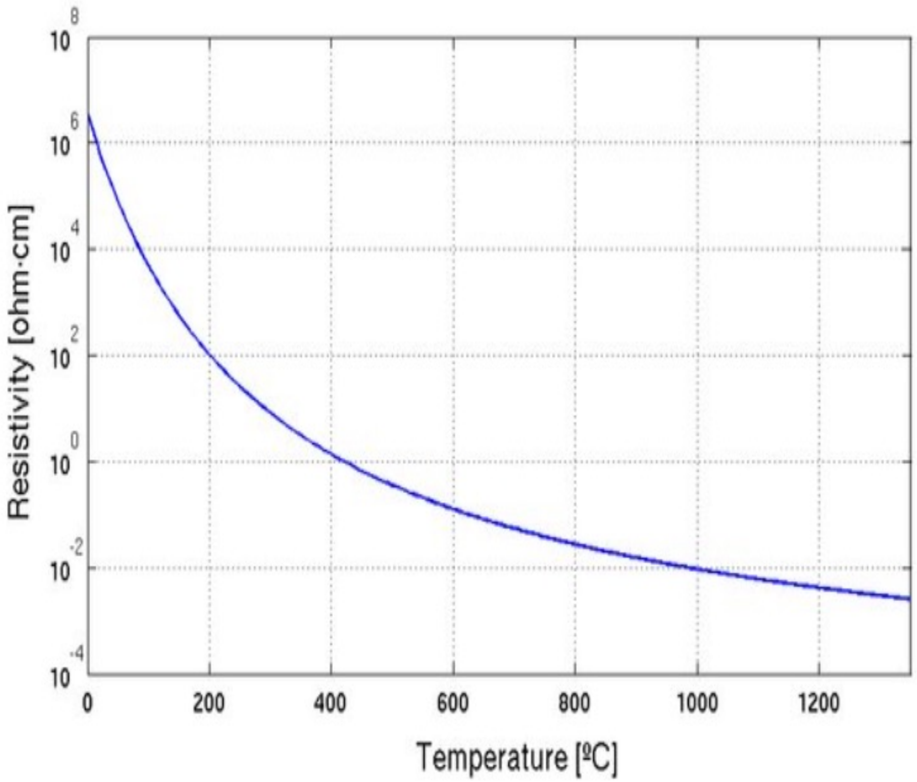
Semiconductors:

In an intrinsic semiconductor, the number of free electrons equals the number of holes.

As the temperature is increased the number of free electrons in the conduction band and holes in valance band increases.

Number of free charge carriers at a fixed temperature also depends on the energy gap of the semiconductor.





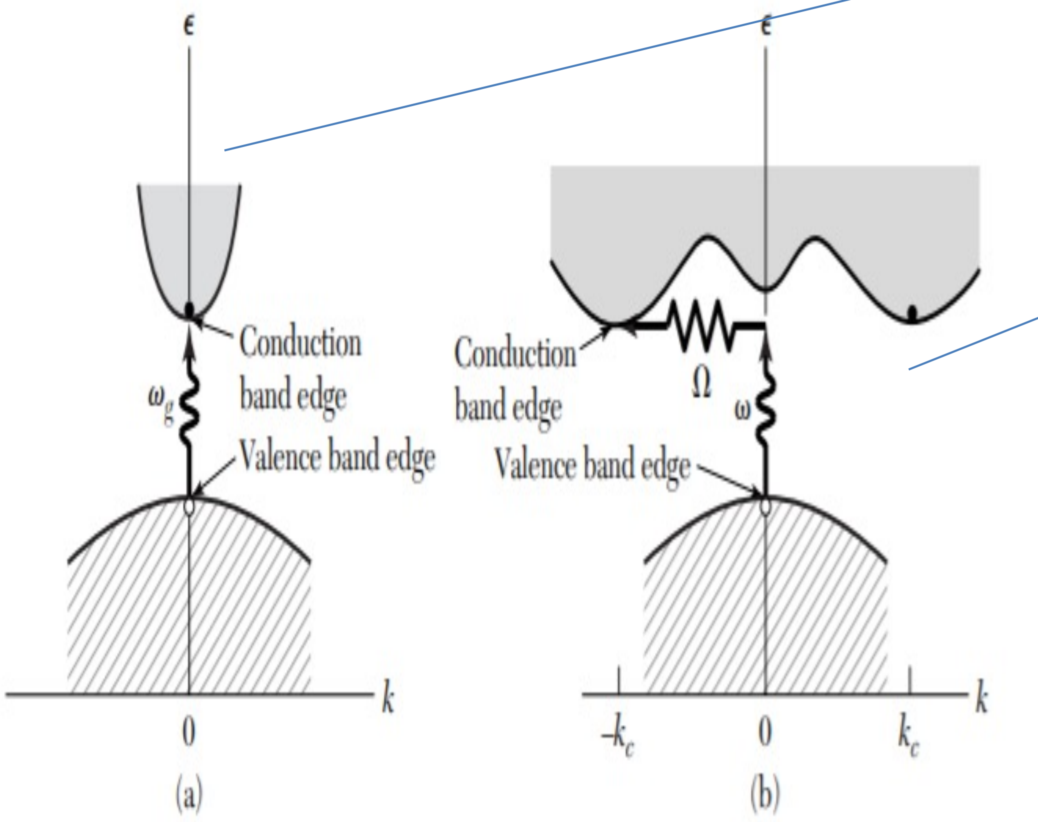
Resistivity behavior of intrinsic silicon material with the temperature.

- For large gap materials number of free electron and holes will lower compared to the material with small band gap at fixed temperature

- Light can also generate free electrons and holes in a semiconductor. Optical: The energy of the photons (hv) must equal or exceed the energy gap of the semiconductor (Eg) .

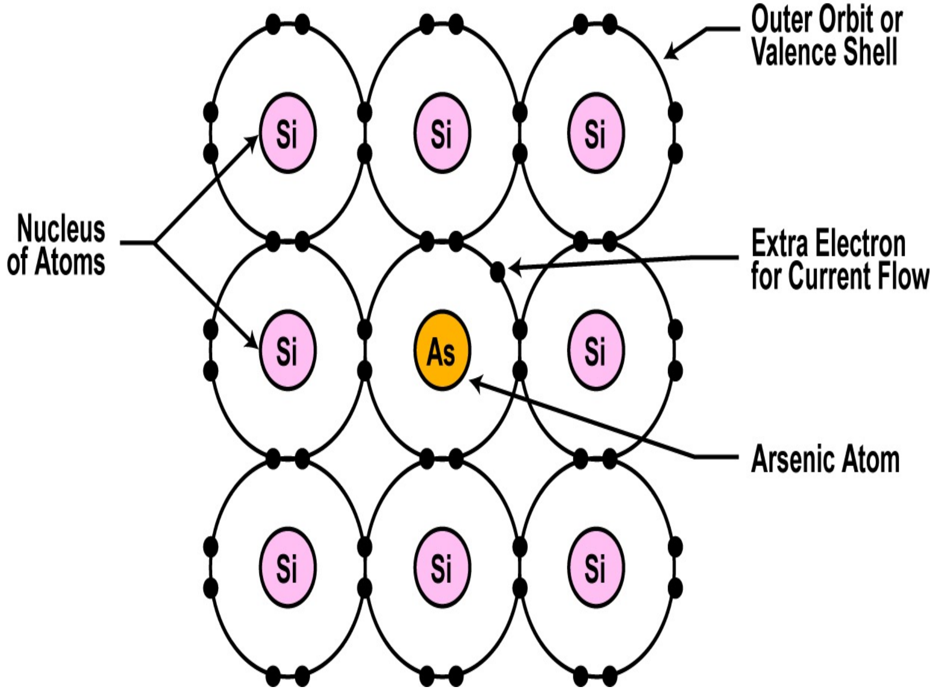
- If hv > Eg , a photon can be absorbed, creating a free electron and a free hole.

Direct and indirect band gap semiconductors:



- In the direct band gap semiconductors, the lowest point of the conduction band occurs at the same value of k as the highest point of the valence band.
- In indirect band gap semiconductors, the lowest of the conduction band and highest point of the valance band both exist at different values of K.
- The indirect transition involves both a photon and a phonon because the band edges of the conduction and valence bands are widely separated in k space as shown in (b)

Semiconductors can become conductor:



Bandgap Values of Several Common Semiconducting Materials

Semiconducting Material	Type	E_g (eV)
Si	Elemental	1.12
Ge	Elemental	0.67
GaP	III-V compound	2.25
GaAs	III-V compound	1.42
CdS	II-VI compound	2.40
ZnTe	II-VI compound	2.26

- An impurity, or element like arsenic, has 5 valence electrons.
- Adding arsenic (doping) will allow four of the arsenic valence electrons to bond with the neighboring silicon atoms.
- The one electron left over for each arsenic atom becomes available to conduct current flow.