



ENGINEERING PHYSICS II (SUBJECT CODE: 303192102)

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Applied Sciences and Humanities

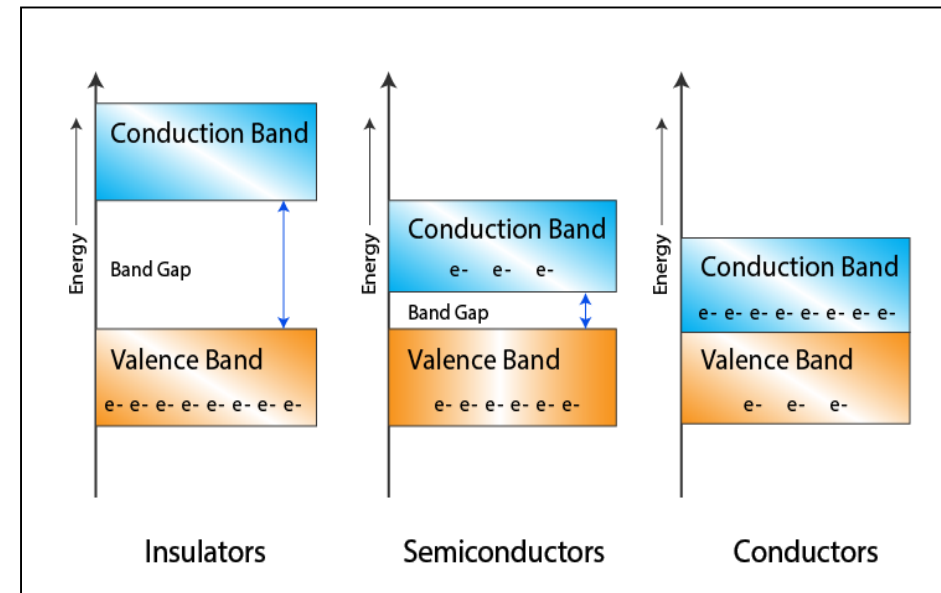


CHAPTER

Band Theory and Semiconductors

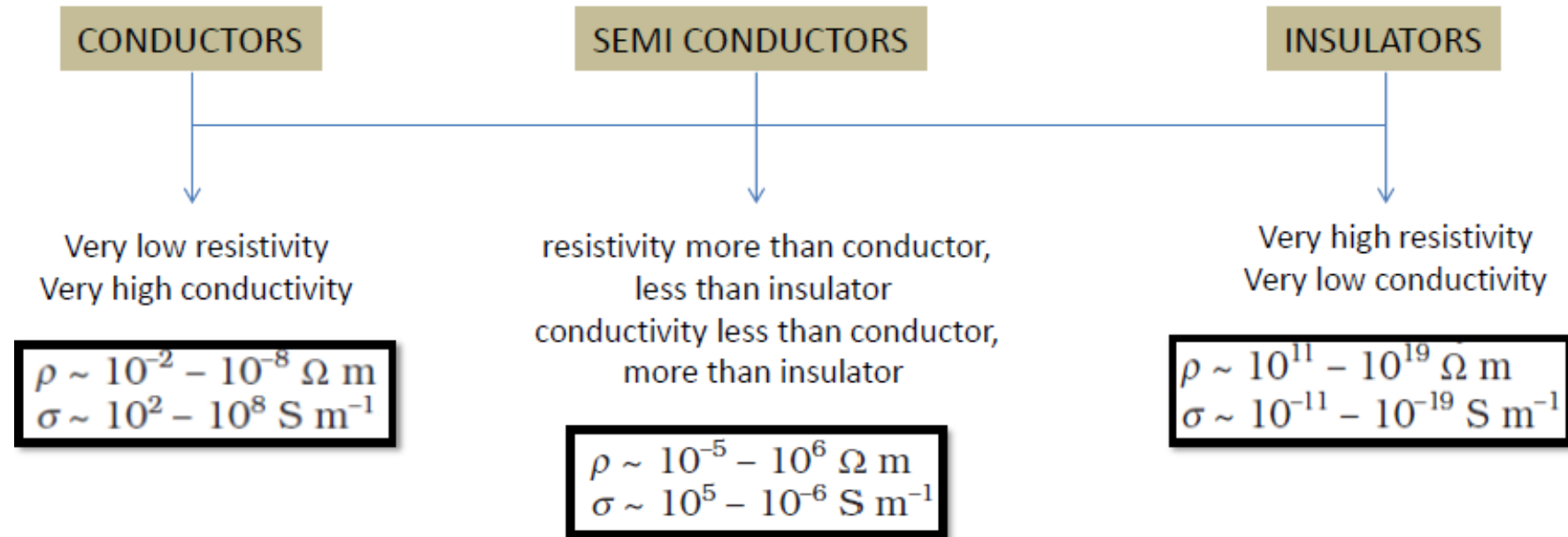
How can we Classify solid Materials

- Solid materials can be classified into three categories based on their electronic structure and properties:
- Conductors, Semiconductors and Insulators.



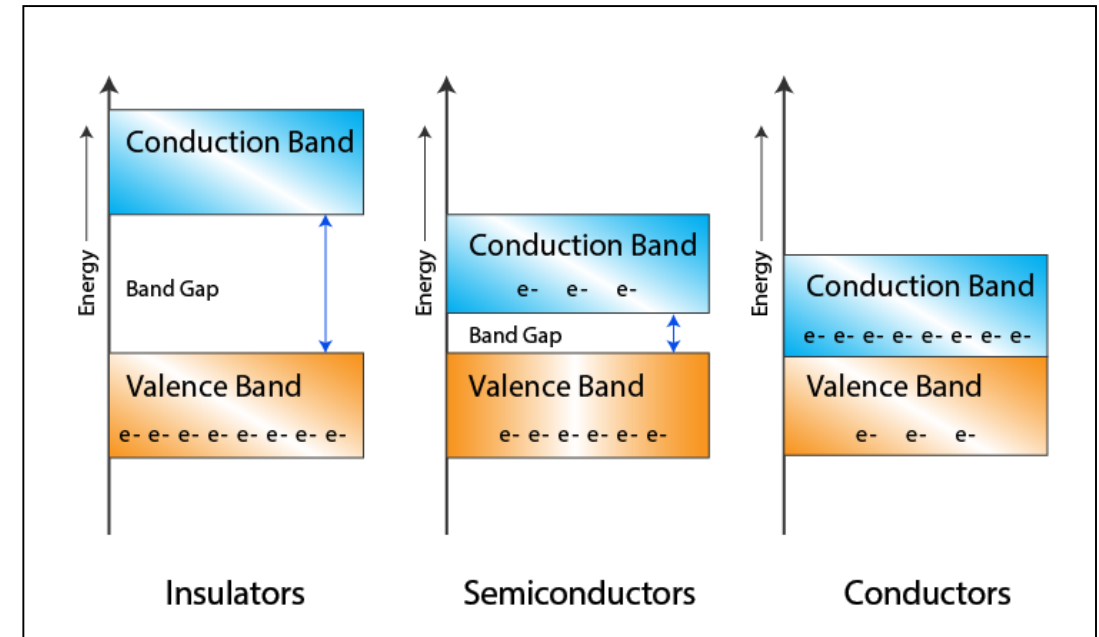
<https://byjus.com/physics/what-are-energy-bands/>

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Concept of Valence band, conduction band and band gap

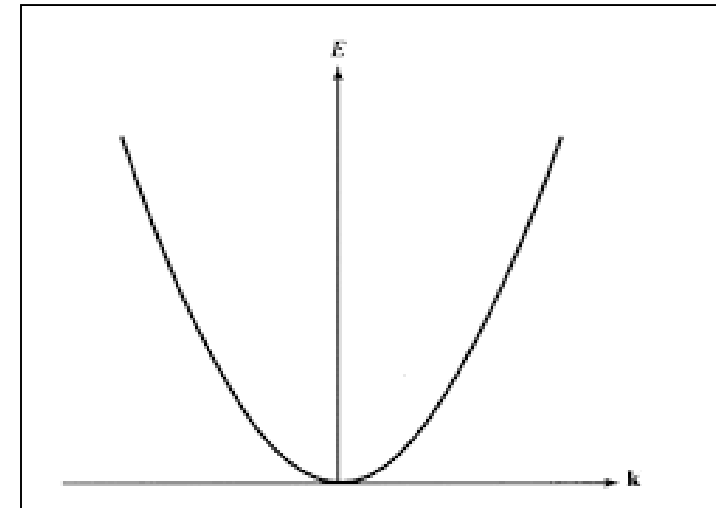
- **Valence band** that contains energy levels of valence electrons which remain in the outermost orbit
- **Conduction band** that contains energy levels of free electrons (conduction electrons)
- **Band gap** is the gap between the top of the valence band and the bottom of the conduction band which does not contain any energy levels.



<https://byjus.com/physics/what-are-energy-bands/>

E K Diagram

- Gives energy-momentum relationship for an electron
- Useful to study band structure
- Gives an idea of band gap
- For a free electron, the relation between energy E and wave vector k is



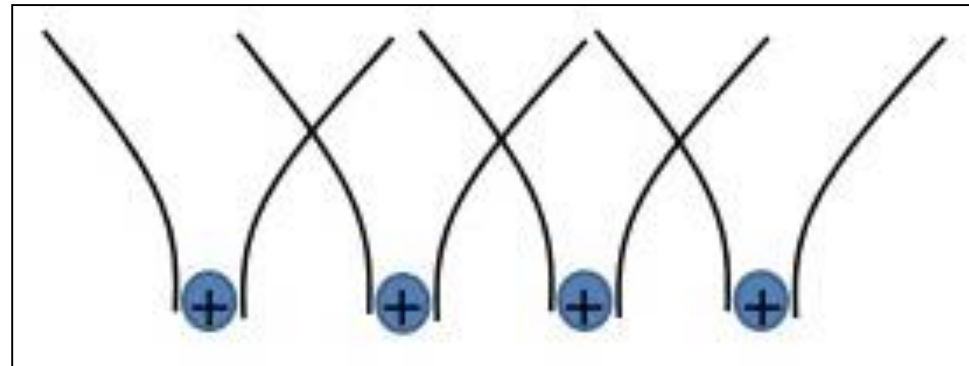
$$E = \frac{\hbar^2 k^2}{2m}$$

- Let us consider electron passing through the periodic arrangement of the atoms of the material

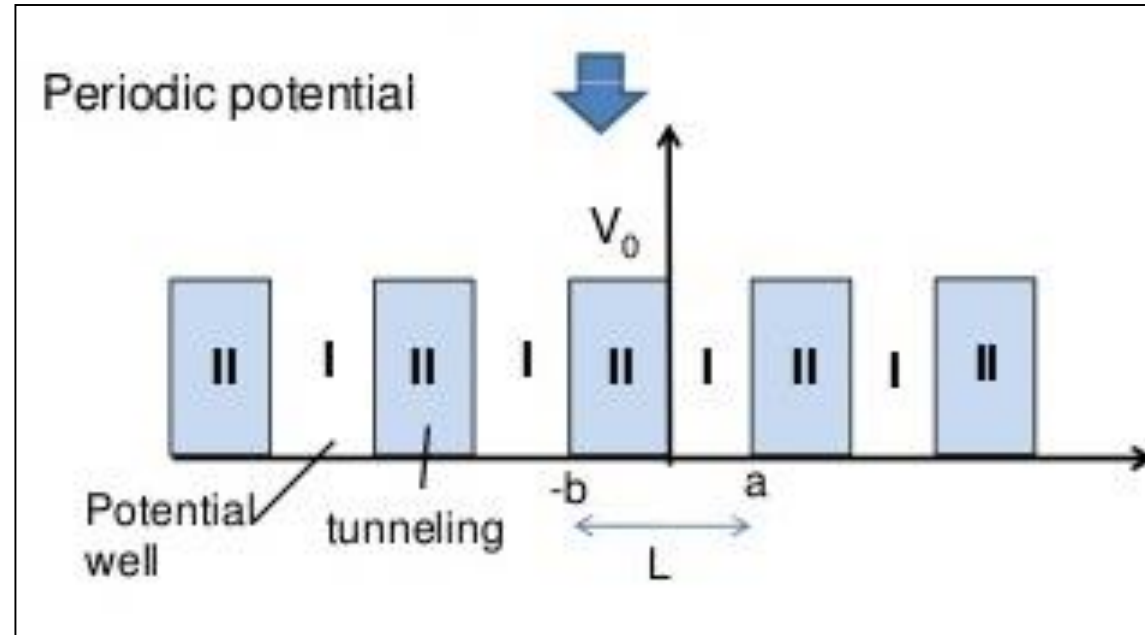
Kronig Penny Model

- Establishes the fact that band gap exists in semiconductors
- Describes motion of electron in one dimensional periodic potential

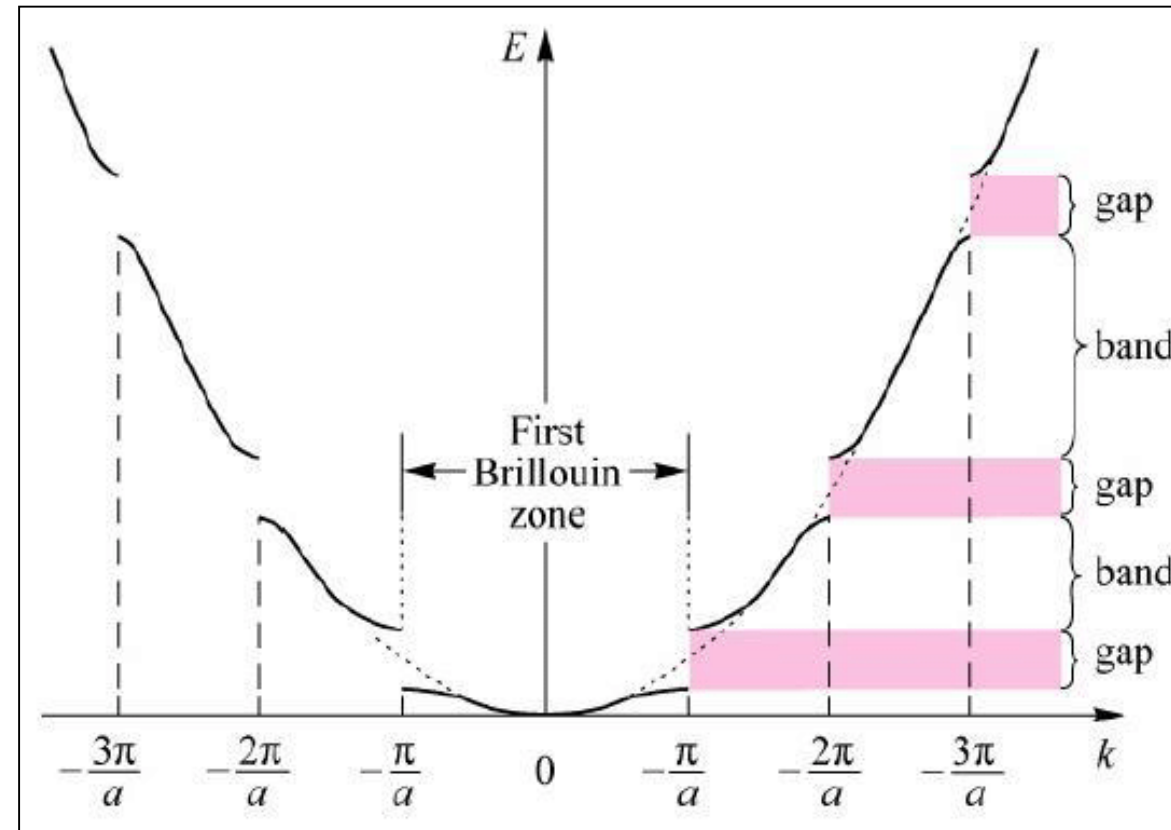
The potentials of adjacent atoms overlap
and gives rise to periodic potential



- Two regions are formed
- Region I of length a
- Region II of length b
- Periodicity is $(a+b)$



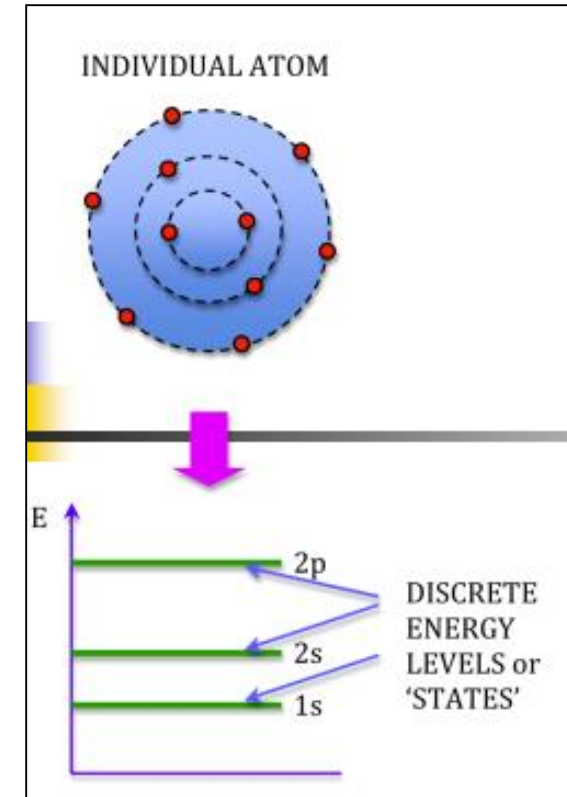
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https://www.researchgate.net/figure/9-Electronic-E-k-diagram-according-to-the-Kronig-Penney-model_fig10_286862888

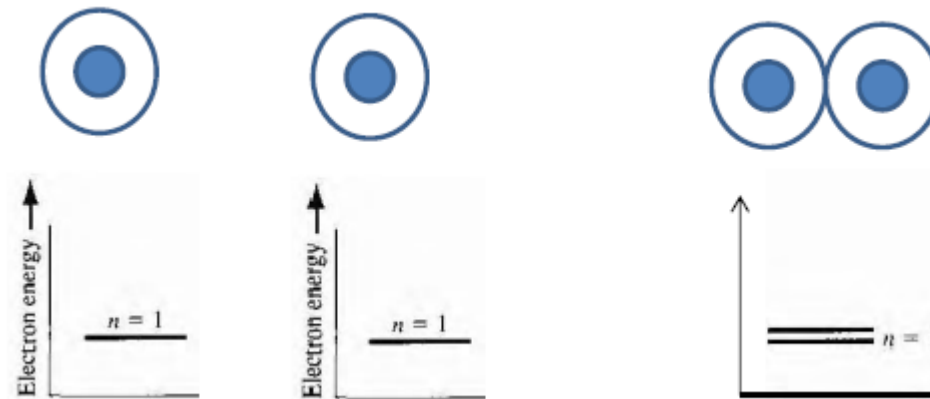
- Why bands are formed in solids?
- Qualitative explanation of how the band gap arises

When atom is single, electrons in discrete orbits will occupy discrete energy levels



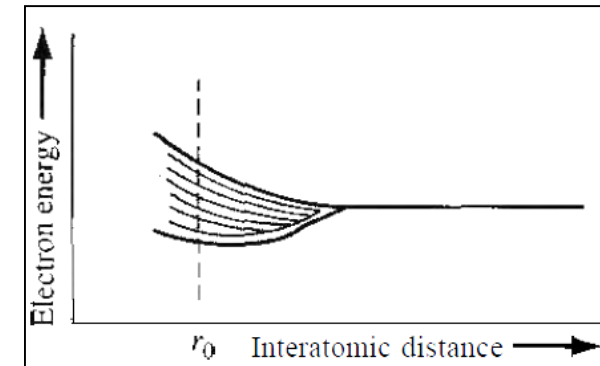
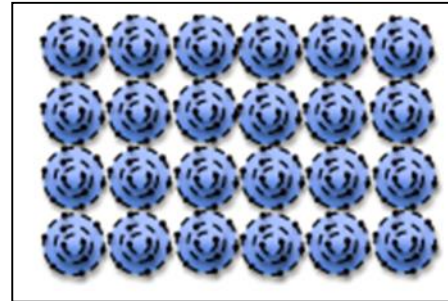
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- Splitting of single energy level into two when atoms containing single electrons are very close



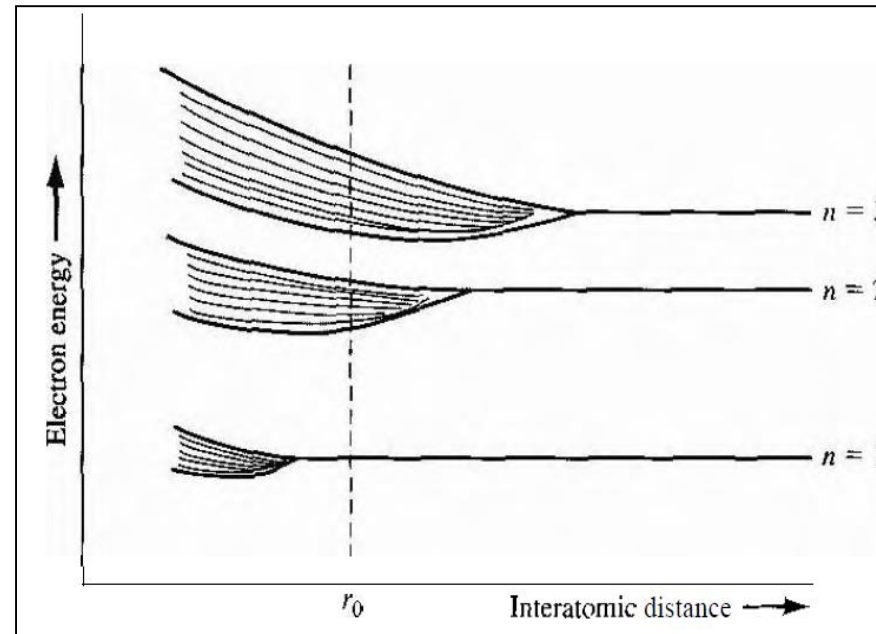
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- If there are N no. of such atoms very close to each other, then energy level $n=1$ will split into N levels.



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- Similarly, if electrons are filled up to 3rd orbit in an atom and when such atoms are brought close to each other, then first $n=3$ level will split because of interaction of outermost electrons, then if the interatomic distance further decreases, electrons of level $n=2$ will start interaction and thus $n=2$ level will split.
- If the interatomic distance further decreases, then electrons of level $n=1$ will also start interacting and the level $n=1$ will also split at very small interatomic distance.



- **Mass of electron under the influence of periodic potential in a material is called effective mass**
- When electron is moving through a crystal, it experiences internal forces due to positive ions and other electrons present. Hence, the original mass of electron seems to change and it is called effective mass of electron.
- **Effective mass can be positive or it can be negative also**

- For free electron,

$$E = \frac{\hbar^2 k^2}{2m}$$

$$\therefore \frac{dE}{dk} = \frac{\hbar^2 2k}{2m} = \frac{\hbar^2 k}{m}$$

$$\therefore \frac{d^2 E}{dk^2} = \frac{\hbar^2}{m}$$

$$\therefore \frac{1}{\hbar^2} \frac{d^2 E}{dk^2} = \frac{1}{m} \dots\dots\dots (1)$$

- The energy of electron near the bottom of the conduction band can be approximated by parabola
- Therefore we can write,

$$E - E_C = c_1 k^2 \text{ (2)}$$

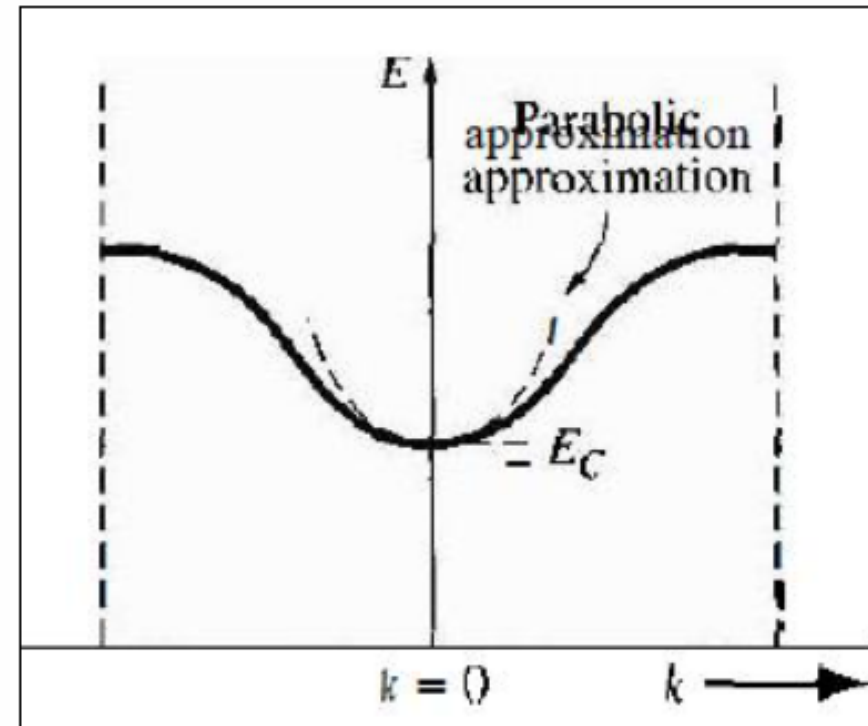
Where E_C is the energy at the bottom of the conduction band

For $k=0$, $E = E_C$

For $k \neq 0$, $E > E_C$

- Therefore c_1 must be positive

- E-k diagram for Conduction band



- Differentiating eq.(2)

$$\frac{dE}{dk} = 2c_1k \quad \therefore \frac{d^2E}{dk^2} = 2c_1 \quad \therefore \frac{1}{\hbar^2} \frac{d^2E}{dk^2} = \frac{1}{\hbar^2} 2c_1 \quad \dots\dots\dots (3)$$

- From eq.(1) and (3)

$$\frac{1}{m} = \frac{1}{\hbar^2} 2c_1 \quad \therefore m = \frac{\hbar^2}{2c_1} \quad \dots\dots\dots (4)$$

- Since c_1 is positive, mass of electron is positive in conduction band.

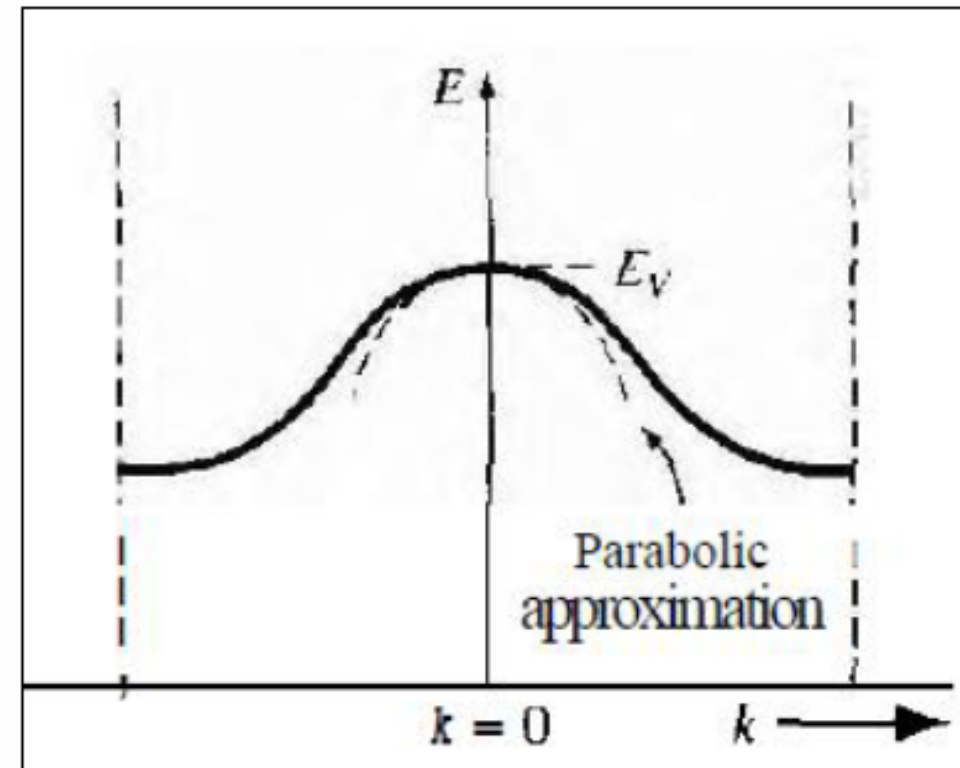
- The energy of electron near the top of the valence band can be approximated by parabola
- Therefore we can write,

$$E_V - E = c_2 k^2 \quad \text{..... (5)}$$

Where E_V is the energy at the top of the valence band

- For $k=0$, $E = E_V$
- For $k \neq 0$, $E < E_V$
- Therefore C_2 must be positive

- E-k diagram for Valence band



- Differentiating eq.(5)

$$-\frac{dE}{dk} = 2c_2k \quad \therefore -\frac{d^2E}{dk^2} = 2c_2 \quad \therefore \frac{1}{\hbar^2} \frac{d^2E}{dk^2} = \frac{-1}{\hbar^2} 2c_2 \quad \dots\dots\dots (6)$$

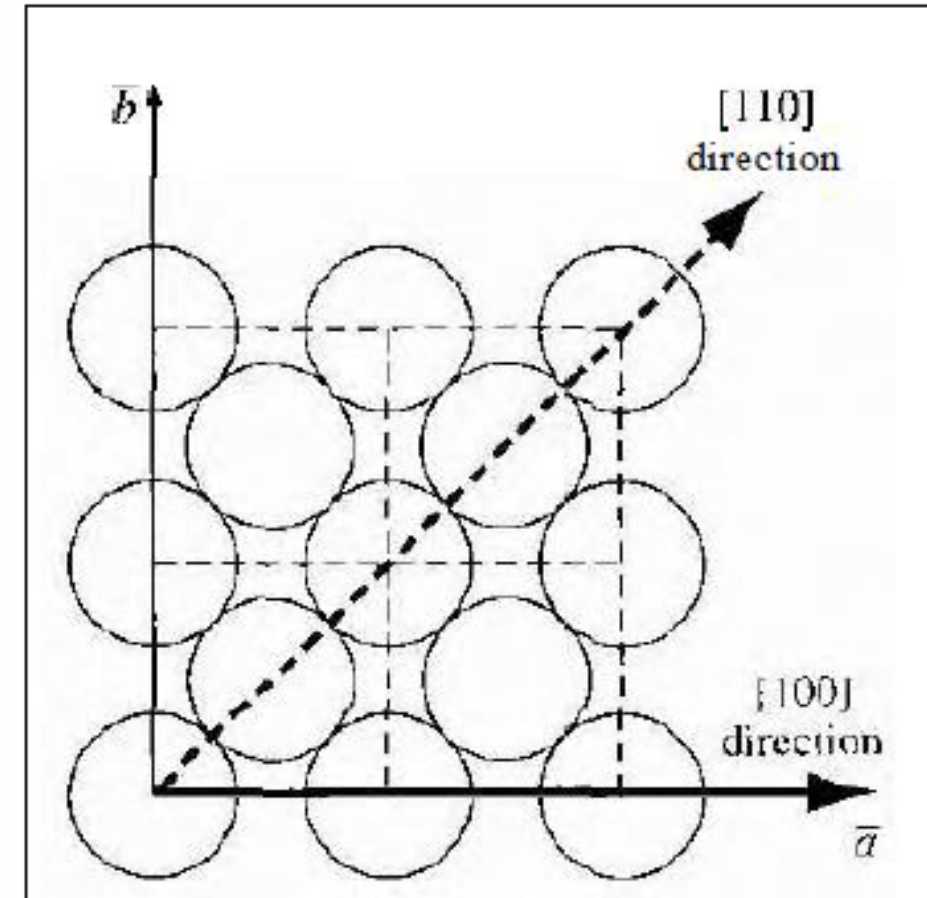
- From eq.(1) and (6)

$$\frac{1}{m} = \frac{-1}{\hbar^2} 2c_2 \quad \therefore m = -\frac{\hbar^2}{2c_2} \quad \dots\dots\dots (7)$$

- Since c_2 is positive, mass of electron is negative in valence band.

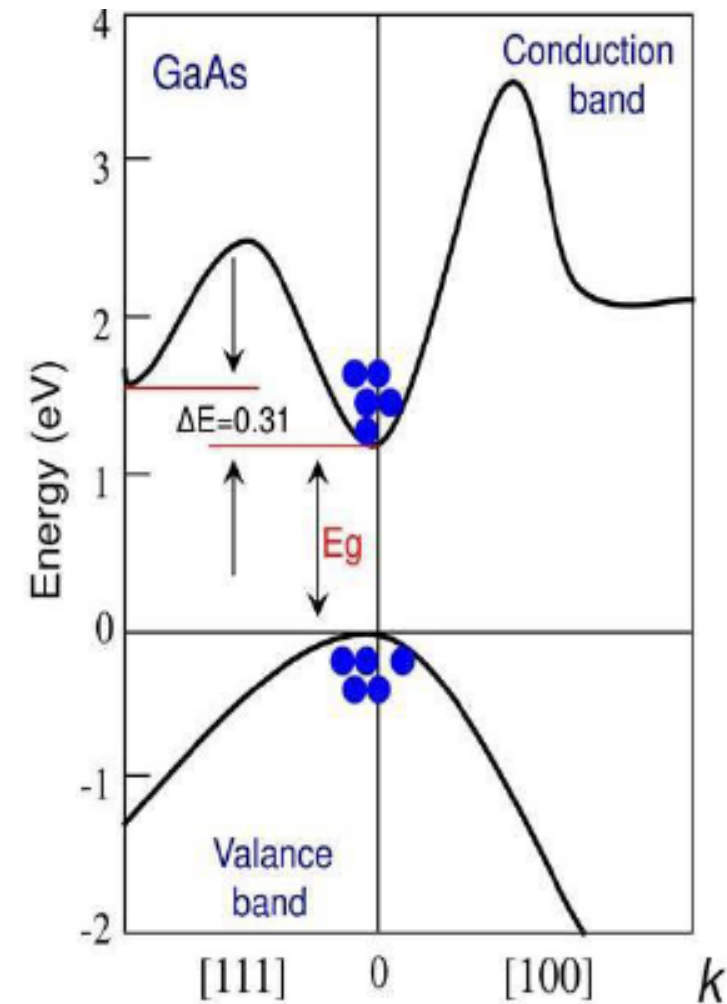
Direct and Indirect band gap materials

- In real three dimensional materials, the spacing between atoms may not be same in all directions
- This gives rise to different band structure in different materials
- Therefore, along different directions, the curvature of E-k diagram will be different.



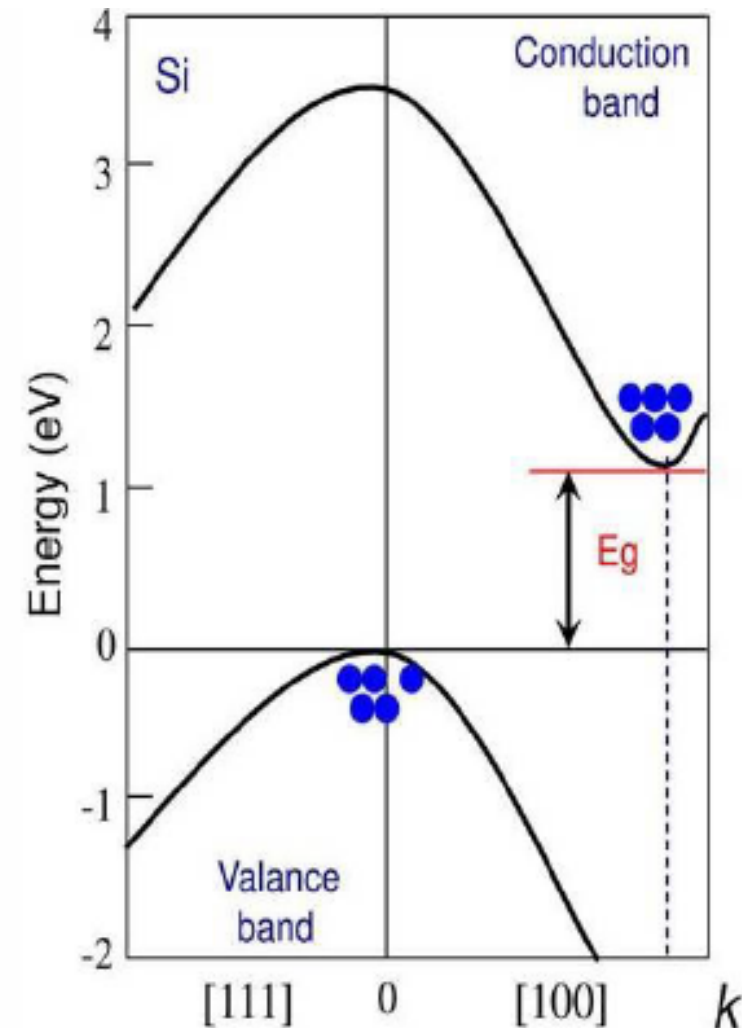
Direct Band Gap Materials

- In such materials, the top of the valence band and the bottom of the conduction band occur at same value of k
- In direct band gap materials, when electron makes transition from conduction band to valence band, the value of k does not change. Hence. The momentum of electron is conserved.
- Direct band gap materials are quite useful in optoelectronic devices like LASER, LED, etc.



Indirect band gap materials

- In such materials, the top of the valence band and the bottom of the conduction band occur at different values of k
- In Indirect band gap materials, when electron makes transition from conduction band to valence band, the value of k changes. Hence, The momentum of electron also changes. Therefore, momentum is not conserved.
- Therefore, electron must interact with lattice in order to adjust its momentum while going from one band to another band.



Examples of Direct and Indirect band gap materials

- Examples of direct bandgap materials include amorphous silicon and some III-V materials such as InAs, GaAs, etc
- Indirect bandgap materials include crystalline silicon and Ge.
- Some III-V materials are indirect bandgap as well, for example Alsb

Application of Direct and Indirect band gap materials

- Transition of electrons from conduction band to valence band takes place vertically in direct band gap semiconductors in which momentum of electron is conserved and there is no need for electron to interact with the lattice. Hence they possess high efficiency for optoelectronic devices.
- Transition of electrons from conduction band to valence band takes place obliquely in indirect band gap semiconductors in which momentum of electron is not conserved and there is a need for electron to interact with the lattice. Hence they possess less efficiency for optoelectronic devices.
- For sources of light like LED or LASER, direct band gap semiconductors must be used.
- For detectors of light like photo diodes, photo transistors , solar cells, indirect band gap semiconductors can be used.

- Density of states is a continuous function of energy in case of conductors
- In case of semiconductors, it is not continuous as there is a band gap
- Variation of density of states as a function of energy is different in valence band and in conduction band

- Density of states for a free electron is given by

$$g(E) = \frac{1}{2\pi^2} \left(\frac{2m}{\hbar^2} \right)^{\frac{3}{2}} E^{\frac{1}{2}} \dots\dots\dots (1)$$

- In eq. (1), E is the energy of a free electron given by

$$E = \frac{\hbar^2}{2m} k^2 \dots\dots\dots (2)$$

- When electron is in conduction band, the equation of its energy is given by,

$$E - E_c = \frac{\hbar^2}{2m} k^2 \dots\dots\dots (3)$$

- Therefore in eq. (1) we can replace E by $E - E_c$

$$\therefore g_c(E) = \frac{1}{2\pi^2} \left(\frac{2m}{\hbar^2} \right)^{\frac{3}{2}} (E - E_c)^{\frac{1}{2}} \dots\dots\dots (4)$$

- Eq. (4) gives density of states in **conduction band**.
- When electron is in valence band, the equation of its energy is given by,

$$E_v - E = \frac{\hbar^2}{2m} k^2 \dots\dots\dots (5)$$

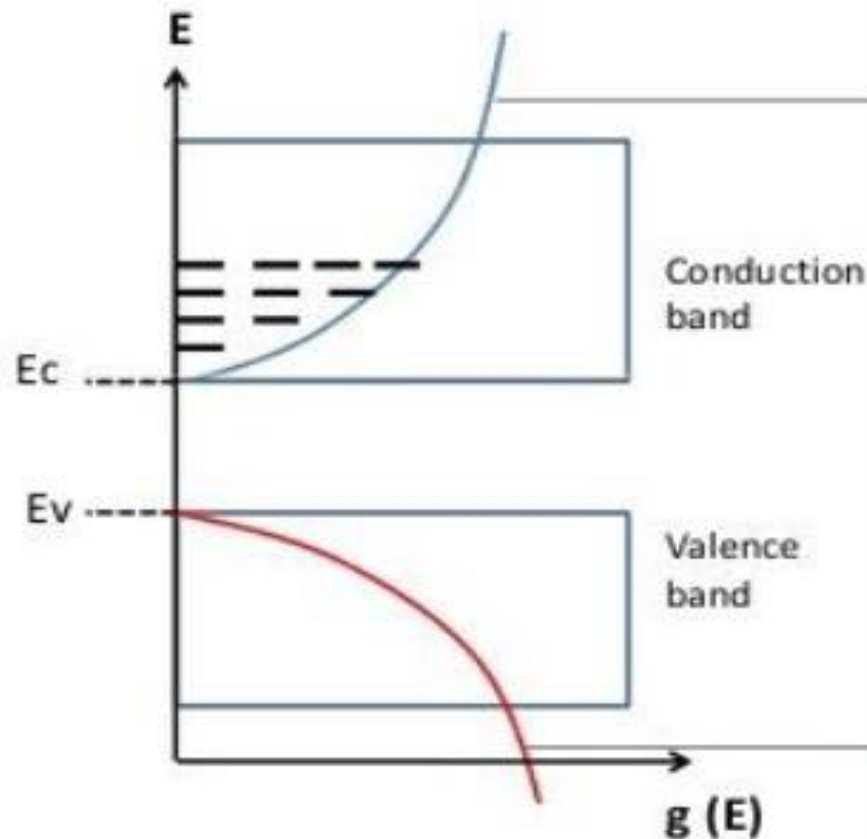
- Therefore in eq. (1) we can replace E by $E_v - E$

$$\therefore g_v(E) = \frac{1}{2\pi^2} \left(\frac{2m}{\hbar^2} \right)^{\frac{3}{2}} (E_v - E)^{\frac{1}{2}} \dots\dots\dots (6)$$

- Eq. (6) gives density of states in **valence band**.

Energy dependence on density of state

Density of state



$$g_c(E) = \frac{1}{2\pi^2} \left(\frac{2m}{\hbar^2} \right)^{\frac{3}{2}} (E - E_c)^{\frac{1}{2}}$$

$$g_v(E) = \frac{1}{2\pi^2} \left(\frac{2m}{\hbar^2} \right)^{\frac{3}{2}} (E_v - E)^{\frac{1}{2}}$$

Charge Carrier Concentration

- How many electrons per unit volume of conduction band?
- How many holes per unit volume of valence band?
- Depends on doping concentration of donor or acceptor impurities
- Decides the conductivity of P-type and N-type materials

Concentration of Electrons in Conduction band

- Occupation probability is given by

$$f_F(E) = \frac{N(E)}{g(E)} \dots\dots\dots (1)$$

- Density of states in conduction band is given by

$$g_c(E) = \frac{1}{2\pi^2} \left(\frac{2m}{\hbar^2} \right)^{\frac{3}{2}} (E - E_c)^{\frac{1}{2}} \dots\dots\dots (2)$$

- From eq. (1) and (2), number of electrons per unit volume per unit energy is given by

$$N(E) = g_c(E) f_F(E) \dots\dots\dots (3)$$

- The number of electrons per unit volume in conduction band can be calculated as

$$n_0 = \int_{E_C}^{\infty} g_c(E) f_F(E) dE \dots\dots\dots (4)$$

where $f_F(E) = \frac{1}{1 + \exp\left(\frac{E - E_F}{KT}\right)} \approx \exp\left(-\frac{(E - E_F)}{KT}\right)$ Assuming $E - E_F \gg KT$

- Substituting eq.(2) in eq. (4)

$$n_0 = \int_{E_c}^{\infty} \frac{1}{2\pi^2} \left(\frac{2m}{\hbar^2} \right)^{\frac{3}{2}} (E - E_c)^{\frac{1}{2}} \exp\left(-\frac{(E - E_F)}{KT}\right) dE$$

$$\therefore n_0 = \frac{1}{2\pi^2} \left(\frac{2m}{\hbar^2} \right)^{\frac{3}{2}} \int_{E_c}^{\infty} (E - E_c)^{\frac{1}{2}} \exp\left(-\frac{(E - E_c)}{KT}\right) \exp\left(-\frac{(E_c - E_F)}{KT}\right) dE$$

$$\therefore n_0 = \frac{1}{2\pi^2} \left(\frac{2m}{\hbar^2} \right)^{\frac{3}{2}} \exp\left(-\frac{(E_c - E_F)}{KT}\right) \int_{E_c}^{\infty} (E - E_c)^{\frac{1}{2}} \exp\left(-\frac{(E - E_c)}{KT}\right) dE$$

- Consider $\eta = \frac{E - E_c}{KT}$ $\therefore d\eta = \frac{dE}{KT}$

$$\therefore n_0 = \frac{1}{2\pi^2} \left(\frac{2m}{\hbar^2} \right)^{\frac{3}{2}} \exp\left(-\frac{(E_c - E_F)}{KT}\right) \int_0^{\infty} (KT)^{\frac{3}{2}} \eta^{\frac{1}{2}} e^{-\eta} d\eta$$

$$\therefore n_0 = \frac{1}{2\pi^2} \left(\frac{2mKT}{\hbar^2} \right)^{\frac{3}{2}} \exp\left(-\frac{(E_C - E_F)}{KT}\right) \frac{\sqrt{\pi}}{2}$$

$$\therefore n_0 = \frac{1}{4} \left(\frac{2mKT}{\pi \hbar^2} \right)^{\frac{3}{2}} \exp\left(-\frac{(E_C - E_F)}{KT}\right)$$

- Taking $m = m_n$ as mass of electron

$$\text{we get, } n_0 = \frac{1}{4} \left(\frac{2m_n KT}{\pi \hbar^2} \right)^{\frac{3}{2}} \exp\left(-\frac{(E_C - E_F)}{KT}\right)$$

$$\therefore n_0 = N_C \exp\left(-\frac{(E_C - E_F)}{KT}\right)$$

Where

$$N_C = \frac{1}{4} \left(\frac{2m_n KT}{\pi \hbar^2} \right)^{\frac{3}{2}}$$

..... (5)

Eq. (5) gives number of electrons per unit volume (concentration) in conduction band.

- Occupation probability is given by

$$f_F(E) = \frac{N(E)}{g(E)} \dots\dots\dots (1)$$

- Density of states in valence band is given by

$$g_V(E) = \frac{1}{2\pi^2} \left(\frac{2m}{\hbar^2} \right)^{\frac{3}{2}} (E_V - E)^{\frac{1}{2}} \dots\dots\dots (2)$$

- From eq. (1) and (2), number of holes per unit volume per unit energy is given by

$$P(E) = g_V(E)(1 - f_F(E)) \quad \dots\dots\dots (3)$$

- The number of holes per unit volume in valence band can be calculated as

$$p_0 = \int_{-\infty}^{E_V} g_V(E)(1 - f_F(E)) dE \quad \dots\dots\dots (4)$$

where

$$1 - f_F(E) = 1 - \frac{1}{1 + \exp\left(\frac{E - E_F}{KT}\right)} = \exp\left(-\frac{(E_F - E)}{KT}\right)$$

- Substituting eq. (2) in eq. (4),

$$p_0 = \int_{-\infty}^{E_V} \frac{1}{2\pi^2} \left(\frac{2m}{\hbar^2} \right)^{\frac{3}{2}} (E_V - E)^{\frac{1}{2}} \exp\left(-\frac{(E_F - E)}{KT}\right) dE$$

$$\therefore p_0 = \frac{1}{2\pi^2} \left(\frac{2m}{\hbar^2} \right)^{\frac{3}{2}} \int_{-\infty}^{E_V} (E_V - E)^{\frac{1}{2}} \exp\left(-\frac{(E_V - E)}{KT}\right) \exp\left(-\frac{(E_F - E_V)}{KT}\right) dE$$

Taking $\eta = \frac{E_V - E}{KT} \quad \therefore d\eta = -\frac{dE}{KT}$

$$\therefore p_0 = \frac{1}{2\pi^2} \left(\frac{2m}{\hbar^2} \right)^{\frac{3}{2}} \exp\left(-\frac{(E_F - E_V)}{KT}\right) \int_0^{\infty} (KT)^{\frac{3}{2}} \eta^{\frac{1}{2}} e^{-\eta} d\eta$$

$$\therefore p_0 = \frac{1}{2\pi^2} \left(\frac{2mKT}{\hbar^2} \right)^{\frac{3}{2}} \exp\left(-\frac{(E_F - E_V)}{KT}\right) \frac{\sqrt{\pi}}{2}$$

$$\therefore p_0 = \frac{1}{4} \left(\frac{2mKT}{\pi \hbar^2} \right)^{\frac{3}{2}} \exp\left(-\frac{(E_F - E_V)}{KT}\right)$$

- Taking $m = m_p$ as mass of hole

$$\begin{aligned} \text{we get, } p_0 &= \frac{1}{4} \left(\frac{2m_p KT}{\pi \hbar^2} \right)^{\frac{3}{2}} \exp\left(-\frac{(E_F - E_V)}{KT}\right) \\ \therefore p_0 &= N_V \exp\left(-\frac{(E_F - E_V)}{KT}\right) \end{aligned} \quad \left. \begin{array}{l} \\ \\ \end{array} \right\} \dots\dots\dots (5)$$

Where,

$$N_V = \frac{1}{4} \left(\frac{2m_p KT}{\pi \hbar^2} \right)^{\frac{3}{2}}$$

- Eq. (5) gives number of holes per unit volume (concentration) in valence band.

Position of Fermi Level in Semiconductors

- Fermi level position is very important factor which characterizes the material as intrinsic, N-type or P-type semiconductor
- Fermi level also changes its position when the material goes out of equilibrium
- Position of fermi level changes when the temperature or doping concentration changes
- When semiconductor device is biased, fermi level again shifts

Intrinsic Semiconductor

- In intrinsic semiconductor, the concentration of electrons in the conduction band is equal to the concentration of holes in the valence band.

$$n_i = p_i \quad \dots\dots\dots (1)$$

Now

$$n_i = \frac{1}{4} \left(\frac{2m_n KT}{\pi \hbar^2} \right)^{\frac{3}{2}} \exp\left(-\frac{(E_C - E_{Fi})}{KT}\right) \quad \dots\dots\dots (2)$$

$$p_i = \frac{1}{4} \left(\frac{2m_p KT}{\pi \hbar^2} \right)^{\frac{3}{2}} \exp\left(-\frac{(E_{Fi} - E_V)}{KT}\right) \quad \dots\dots\dots (3)$$

Where E_{Fi} is fermi energy in intrinsic semiconductor

- Substituting eq. (2) and (3) in eq. (1)

$$\frac{1}{4} \left(\frac{2m_n KT}{\pi \hbar^2} \right)^{\frac{3}{2}} \exp\left(-\frac{(E_C - E_{Fi})}{KT}\right) = \frac{1}{4} \left(\frac{2m_p KT}{\pi \hbar^2} \right)^{\frac{3}{2}} \exp\left(-\frac{(E_{Fi} - E_V)}{KT}\right)$$

$$\therefore \exp\left(-\frac{(E_C - E_{Fi})}{KT}\right) = \exp\left(-\frac{(E_{Fi} - E_V)}{KT}\right)$$

$$\therefore -\frac{(E_C - E_{Fi})}{KT} = -\frac{(E_{Fi} - E_V)}{KT}$$

$$\therefore E_{Fi} - E_C = -E_{Fi} + E_V$$

$$\therefore 2 E_{Fi} = E_C + E_V \quad \therefore \quad E_{Fi} = \frac{E_C + E_V}{2} \quad \dots\dots\dots (4)$$

- From eq. (4), we can say that fermi energy level in intrinsic semiconductor lies exactly in the middle of the band gap.

$$\text{electron concentration, } n = N_C \exp\left(-\frac{(E_C - E_F)}{KT}\right) \dots\dots\dots (1)$$

$$\therefore \frac{n}{N_C} = \exp\left(-\frac{(E_C - E_F)}{KT}\right)$$

$$\therefore \ln\left(\frac{n}{N_C}\right) = -\frac{(E_C - E_F)}{KT}$$

$$\therefore \frac{(E_C - E_F)}{KT} = -\ln\left(\frac{n}{N_C}\right)$$

$$\therefore \frac{(E_C - E_F)}{KT} = \ln\left(\frac{N_C}{n}\right)$$

$$\therefore E_C - E_F = KT \ln\left(\frac{N_C}{n}\right) \dots\dots\dots (2)$$

$$\text{hole concentration, } p = N_V \exp\left(-\frac{(E_F - E_V)}{KT}\right) \dots\dots\dots (3)$$

$$\therefore \frac{p}{N_V} = \exp\left(-\frac{(E_F - E_V)}{KT}\right)$$

$$\therefore \ln\left(\frac{p}{N_V}\right) = -\frac{(E_F - E_V)}{KT}$$

$$\therefore \frac{(E_F - E_V)}{KT} = -\ln\left(\frac{p}{N_V}\right)$$

$$\therefore \frac{(E_F - E_V)}{KT} = \ln\left(\frac{N_V}{p}\right)$$

$$\therefore E_F - E_V = KT \ln\left(\frac{N_V}{p}\right) \dots\dots\dots (4)$$

- Thus we have,

$$E_C - E_F = KT \ln\left(\frac{N_C}{n}\right)$$

$$E_F - E_V = KT \ln\left(\frac{N_V}{p}\right)$$

- For intrinsic semiconductor,

$$n = p \quad \text{Therefore,} \quad E_C - E_F = E_F - E_V$$

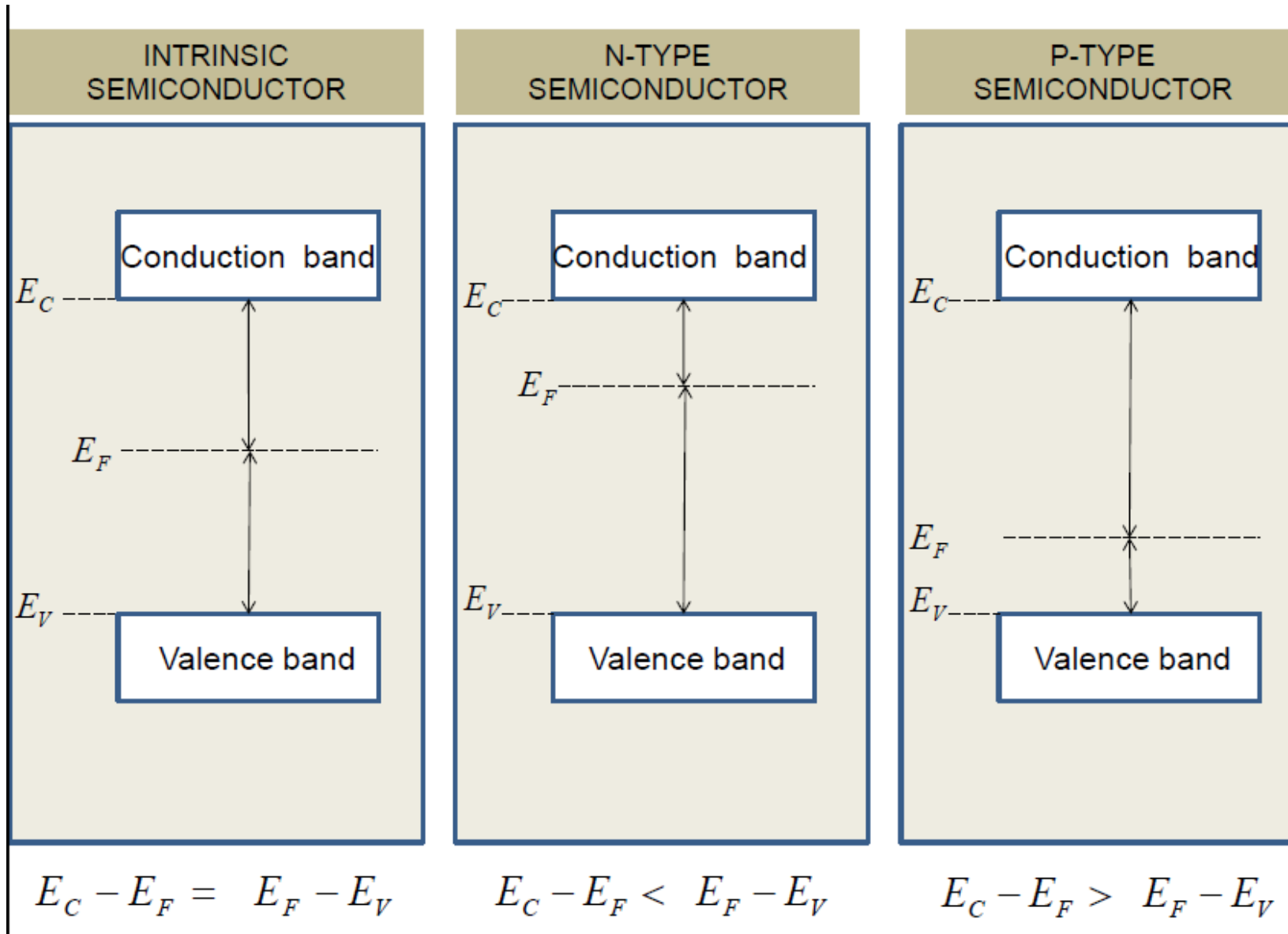
- For N-type semiconductor,

$$n > p \quad \text{Therefore,} \quad E_C - E_F < E_F - E_V$$

- For P-type semiconductor,

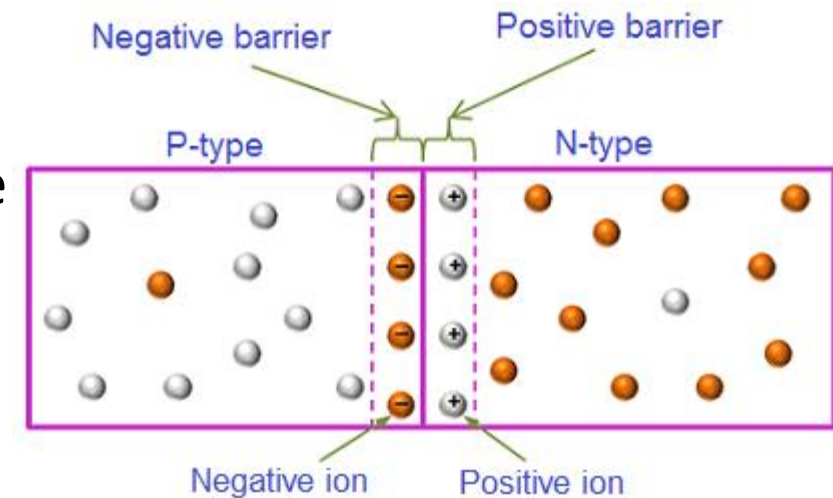
$$n < p \quad \text{Therefore,} \quad E_C - E_F > E_F - E_V$$

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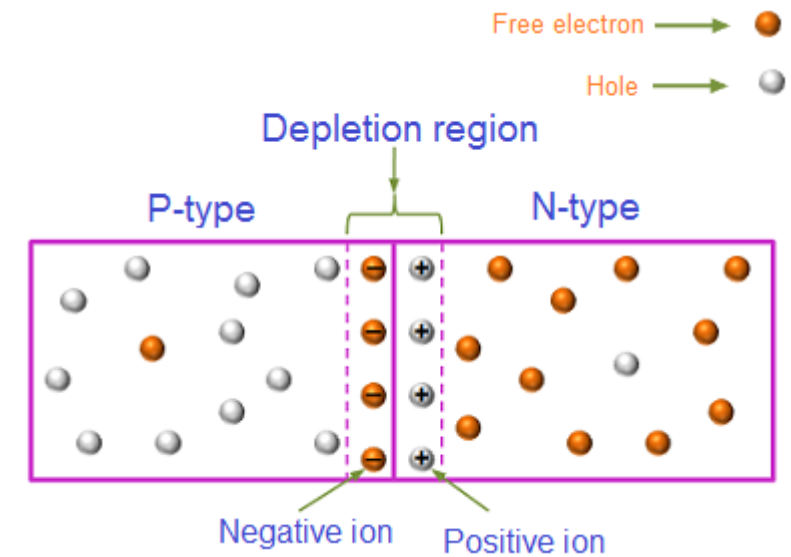
P N Junction

- In n-type region, large number of free electrons is present & get repelled from each other. So, move from a high concentration n-region to a low concentration p-region.
- Near pn-junction free electrons & holes are close to each other.
- Coulombs law: Free electrons from n-side attracted towards the holes at p-side. So, the free electrons move from n-side to p-side. Holes move from p-side to n-side.



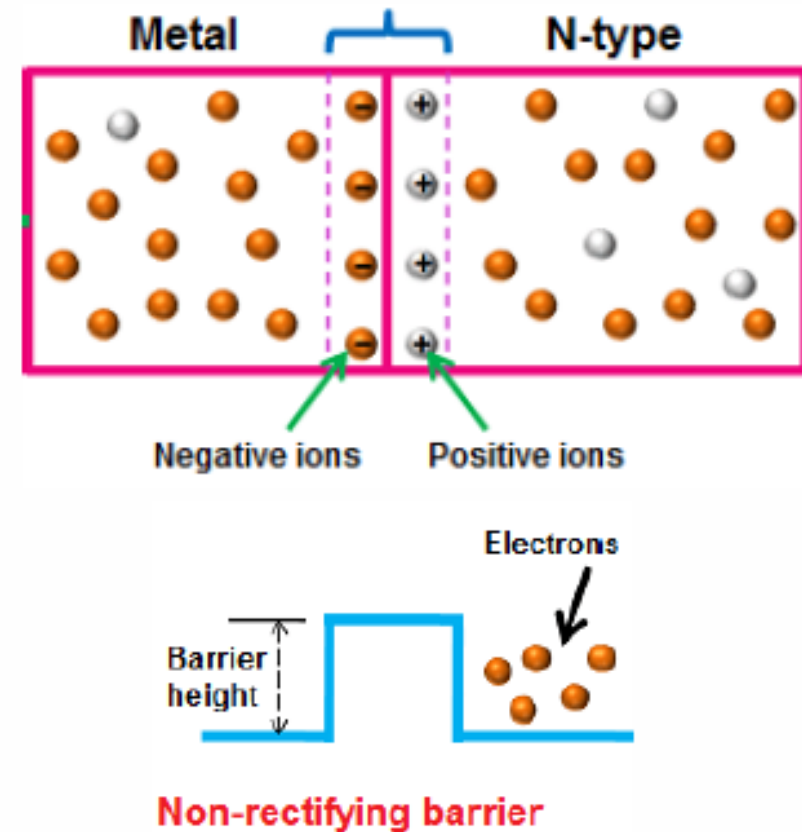
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- Free electrons cross pn-junction & fill holes in p-side atoms.
- The p-atom/side turns with more electron than protons become a negative ion (charge).
- Each free electron that left the parent n-atom turns n-side as positive ion (charge).
- The net negative charge at p-side prevents further flow of free electrons crossing pn-junction (because the negative charge present at the p-side repels the free electrons).
- Similarly, the net positive charge at n-side prevents further flow of holes from p-side to n-side.
- Barrier: Depletion region or depletion zone or depletion layer



Ohmic Junction

- Ohmic junction is formed when a metal is in contact with another metal or with the heavily doped semiconductor.
- Such junctions are usually **non-rectifying**
- When electrons diffuse from heavily doped semiconductor to metal, a very narrow depletion region is formed which does not have rectifying capability

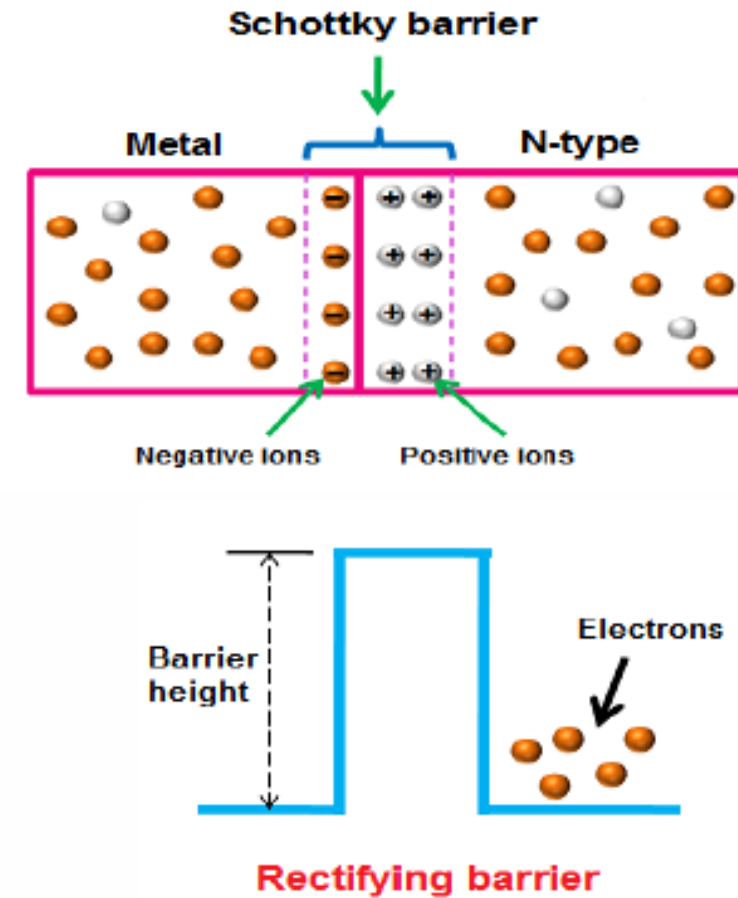


- When electrons diffuse from heavily doped N-type semiconductor to metal, positive ions are produced in N-type semiconductor and negative ions are produced in metal.
- now metal as well as heavily doped N-type semiconductor both have high density of states and hence the atoms from narrow region of N-type semiconductor will lose electrons and the atoms from narrow region of metal will gain electrons.
- Because of this the depletion region is thin within N-type semiconductor as well as within metal.

- Thus, the overall depletion region across the junction is extremely narrow (negligible) and hence the potential barrier height is also very less so that electrons can easily overcome this barrier.
- Ohmic junction can conduct in both the directions due to very less contact potential and it is unable to rectify the A.C. signal. Therefore, it is known as non rectifying junction or Ohmic junction.

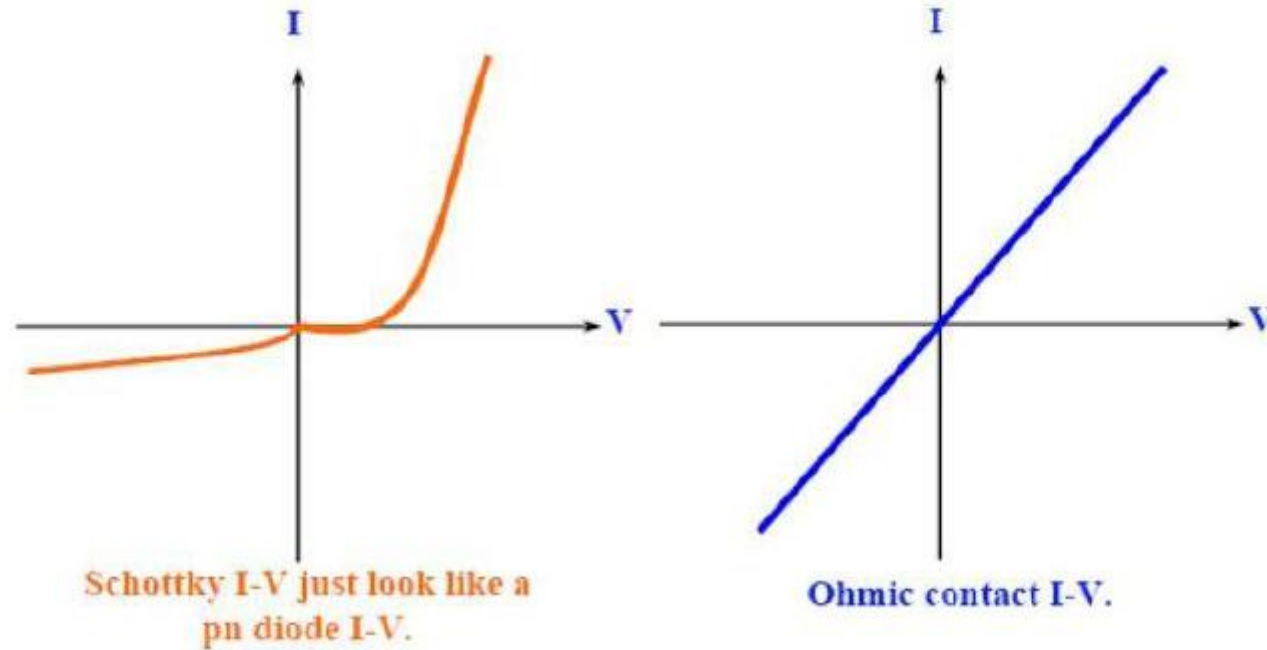
Schottky Junction

- Schottky junction is formed when a metal is in contact with the lightly doped semiconductor.
- When electrons diffuse from N-type semiconductor to metal, positive ions are produced in N-type semiconductor and negative ions are produced in metal.
- metals usually have high density of states (large no. of available states per unit volume) and hence more electrons can be accommodated within less volume.



- Hence the atoms from wider region of N-type semiconductor will lose electrons and the atoms from narrow region of metal will gain electrons.
- Therefore the depletion region is thick within N-type semiconductor and thin within metal
- Because of the depletion region, a potential barrier is developed across the junction which is sufficiently high so that electrons cannot overcome this barrier.
- When external voltage source is connected in forward bias, this barrier height will decrease and the current will be conducted through the junction whereas under reverse bias, this barrier height will increase and the current will not be conducted through the junction. Hence, this junction becomes rectifying junction.

I-V Characteristics of Ohmic and Schottky Junction



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