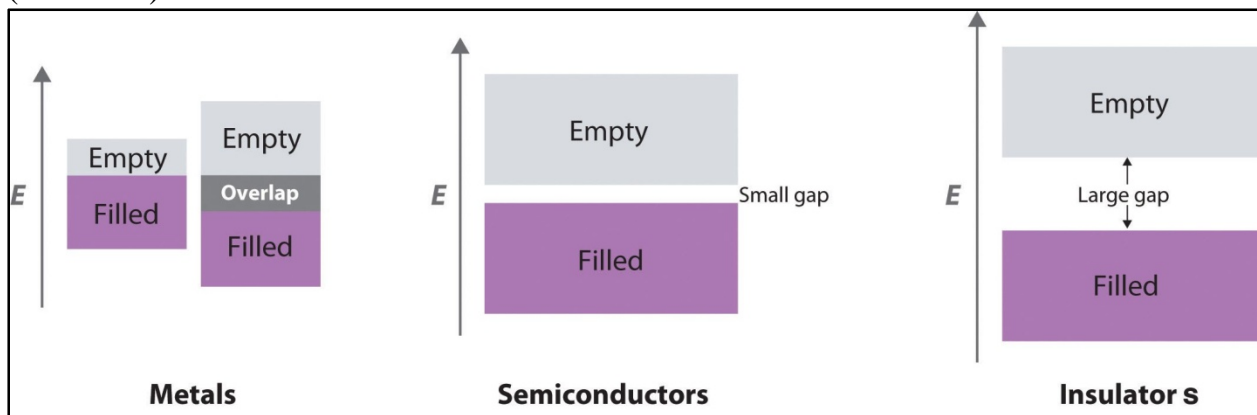


UNIT-II

2.1 Energy bands in intrinsic and extrinsic silicon

Every solid has its own characteristic energy band structure. This variation in band structure is responsible for the wide range of electrical characteristics observed in various materials. For electrons to experience acceleration in an applied electric field, they must be able to move into new energy states. This implies there must be empty states (allowed energy states which are not already occupied by electrons) available to the electrons. For example, if relatively few electrons reside in an empty band, ample unoccupied states are available into which the electrons can move. On the other hand, the silicon band structure is such that the valence band is completely filled with electrons at 0 K and the conduction band is empty. There can be no charge transport within the valence band, since no empty states are available into which electrons can move. There are no electrons in the conduction band, so no charge transport can take place there either. Thus silicon has a high resistivity typical of insulators.

Semiconductor materials at 0 K have basically the same structure as insulators—a filled valence band separated from an empty conduction band by a band gap containing no allowed energy states. The difference lies in the size of the band gap E_g , which is much smaller in semiconductors than in insulators. For example, the semiconductor Si has a band gap of about 1.1 eV compared with 5 eV for diamond (insulator).

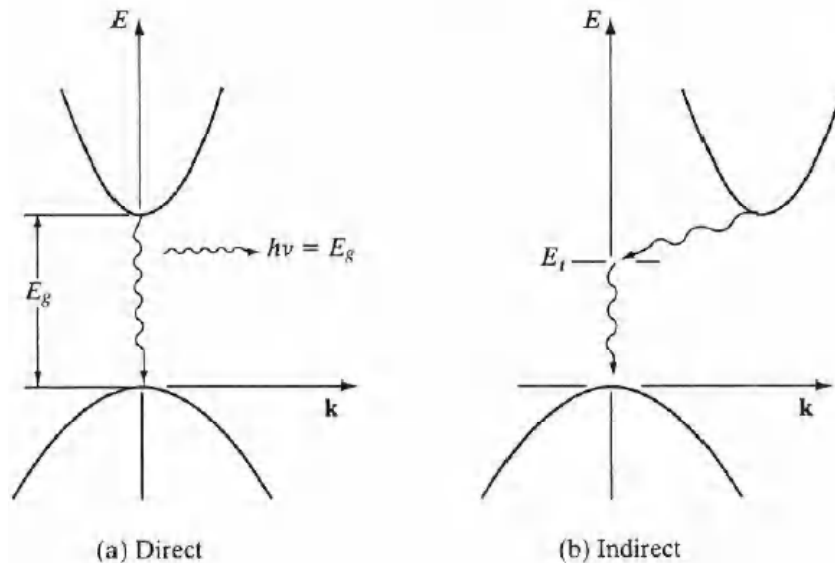


The relatively small band gaps of semiconductors allow for excitation of electrons from the lower (valence) band to the upper (conduction) band by reasonable amounts of thermal or optical energy. For example, at room temperature a semiconductor with a 1-eV band gap will have a significant number of electrons excited thermally across the energy gap into the conduction band, whereas an insulator with $E_g = 10 \text{ eV}$ will have a negligible number of such excitations.

Thus an important difference between semiconductors and insulators is that the number of electrons available for conduction can be increased greatly in semiconductors by thermal or optical energy.

In metals the bands either overlap or are only partially filled. Thus electrons and empty energy states are intermixed within the bands so that electrons can move freely under the influence of an electric field.

Direct and Indirect Semiconductors



In direct band gap semiconductors, minimum in the conduction band and maximum in the valence band lies in the same k -value (e.g., GaAs). On the other hand, indirect semiconductor has its valence band maximum at a different value of k than its conduction band minimum (e.g., Si). Thus an electron making a smallest-energy transition from the conduction band to the valence band in GaAs can do so without a change in k value; on the other hand, a transition from the minimum point in the Si conduction band to the maximum point of the valence band requires some change in k . In a direct semiconductor such as GaAs, an electron in the conduction band can fall to an empty state in the valence band, giving off the energy difference E_g as a photon of light. On the other hand, an electron in the conduction band minimum of an indirect semiconductor such as Si cannot fall directly to the valence band maximum but must undergo a momentum change as well as changing its energy. For example, it may go through some defect state within the band gap. In an indirect transition which involves a change in k , part of the energy is generally given up as heat to the lattice rather than as an emitted photon. This difference between direct and indirect band structures is very important for deciding which semiconductors can be used in devices requiring light

output. For example, semiconductor light emitters and lasers generally must be made of materials capable of direct band-to-band transitions or of indirect materials with vertical transitions between defect states.

CHARGE CARRIERS IN SEMICONDUCTORS

As the temperature of a semiconductor is raised from 0 K, some electrons in the valence band receive enough thermal energy to be excited across the band gap to the conduction band. The result is a material with some electrons in an empty conduction band and some unoccupied states in an otherwise filled valence band.

For convenience, an empty state in the valence band is referred to as a *hole*. If the conduction band electron and the hole are created by the excitation of a valence band electron to the conduction band, they are called an *electron-hole pair* (abbreviated EHP).

After excitation to the conduction band, an electron is surrounded by a large number of unoccupied energy states. For example, the equilibrium number of electron-hole pairs in pure Si at room temperature is only about 1.5×10^{10} EHP/cm³, compared to the Si atom density of 5×10^{22} atoms/cm³. Thus the few electrons in the conduction band are free to move about via the many available empty states.

Effective Mass

In solid state physics, a particle's effective mass (often denoted m^*) is the mass that it seems to have when responding to forces, or the mass that it seems to have when interacting with other identical particles in a thermal distribution.

One of the results from the band theory of solids is that the movement of particles in a periodic potential, over long distances larger than the lattice spacing, can be very different from their motion in a vacuum.

The effective mass is a quantity that is used to simplify band structures by modeling the behavior of a free particle with that mass. For some purposes and some materials, the effective mass can be considered to be a simple constant of a material. In general, however, the value of effective mass depends on the purpose for which it is used, and can vary depending on a number of factors.

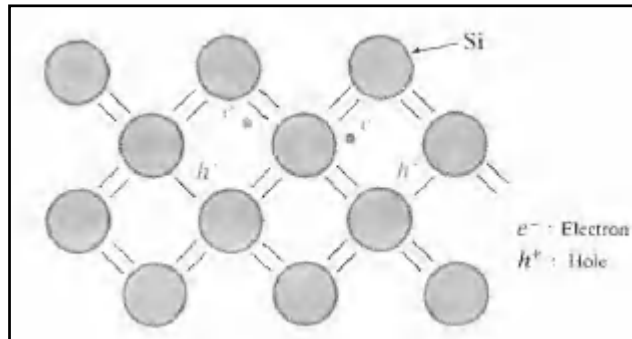
Intrinsic vs Extrinsic Materials:

Intrinsic Semiconductors:

A perfect semiconductor crystal with no impurities or lattice defects is called an *intrinsic* semiconductor.

In such material there are no charge carriers at 0 K, since the valence band is filled with electrons and the conduction band is empty. At higher temperatures electron-hole pairs are generated as valence band electrons are excited thermally across the

band gap to the conduction band. These EHPs are the only charge carriers in intrinsic material.



Electron-hole pairs in the covalent bonding model or the Si crystal.

The generation of EHPs can be visualized in a qualitative way by considering the breaking of covalent bonds in the crystal lattice (as shown in above Fig.). If one of the Si valence electrons is broken away from its position in the bonding structure such that it becomes free to move about in the lattice, a conduction electron is created and a broken bond (hole) is left behind. The energy required to break the bond is the band gap energy E_g . This model helps in visualizing the physical mechanism of EHP creation, but the energy band model is more productive for purposes of quantitative calculation.

Since the electrons and holes are created in pairs, the conduction band electron concentration n (electrons per cm^3) is equal to the concentration of holes in the valence band p (holes per cm^3)(**only for intrinsic**). Each of these intrinsic carrier concentrations is commonly referred to as n_i . Thus *for intrinsic material*

$$n=p=n_i$$

At a given temperature there is a certain concentration of electron-hole pairs n_i . Obviously, if a steady state carrier concentration is maintained, there must be recombination of EHPs at the same rate at which they are generated.

Recombination occurs when an electron in the conduction band makes a transition (direct or indirect) to an empty state (hole) in the valence band, thus annihilating the pair. If we denote the generation rate of EHPs as g_i (EHP/ cm^3 -s) and the recombination rate as r_i , equilibrium requires that:

$$r_i=g_i$$

Each of these rates is temperature dependent. For example, $g_i(T)$ increases when the temperature is raised, and **a new carrier concentration n_i** , is established such that the higher recombination rate $r_i(T)$ just balances generation. At any temperature, we can predict that the rate of recombination of electrons and holes is proportional to the equilibrium concentration of electrons n_0 and the concentration of holes p_0 :

$$r_i=\alpha_r n_0 p_0=\alpha_r n_i^2=g_i$$

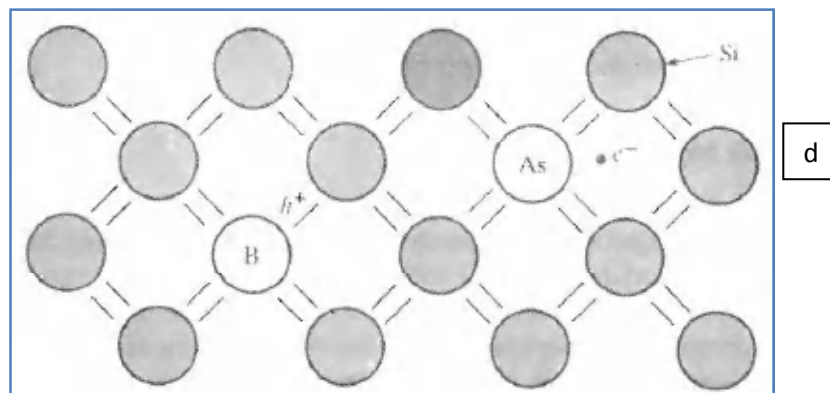
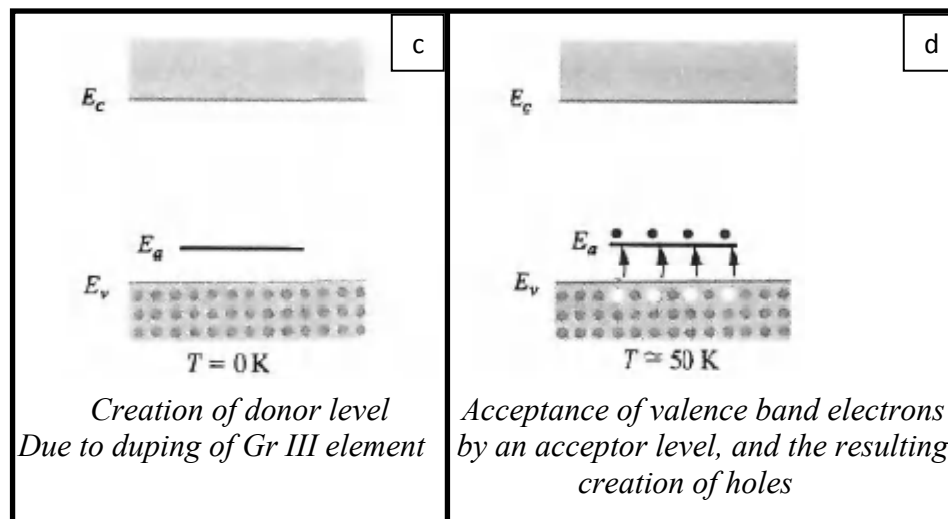
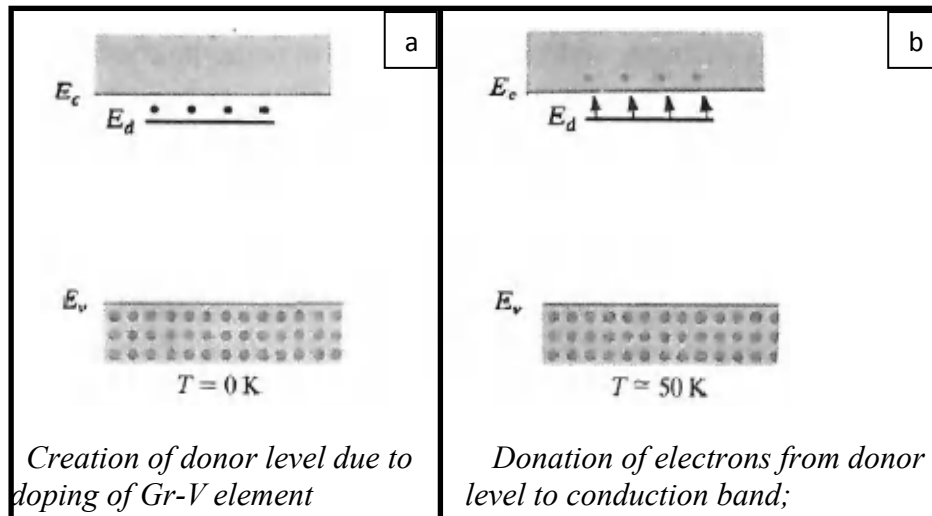
The factor α_r is a constant of proportionality which depends on the particular mechanism by which recombination takes place.

Extrinsic Semiconductors:

In addition to the intrinsic carriers generated thermally, it is possible to create carriers in semiconductors by purposely introducing impurities into the crystal. This process, called *doping*, is the most common technique for varying the conductivity of the semiconductors. By doping, a crystal can be altered so that it has a predominance of either electrons or holes. Thus there are two types of doped semiconductors, n-type (mostly electrons) and p-type (mostly holes). When a crystal is doped such that the equilibrium carrier concentrations n_0 and p_0 are different from the intrinsic carrier concentration n_i , the material is said to be *extrinsic*.

When impurities are introduced into an otherwise perfect crystal, additional levels are created in the energy band structure, usually within the band gap. For example, an impurity from column V of the periodic table (P, As, and Sb) introduces an energy level very near the conduction band in Ge or Si. This level is filled with electrons at 0 K, and very little thermal energy is required to excite these electrons to the conduction band. At about 50-100 K, virtually all of the electrons in the impurity level are "donated" to the conduction band. Such an impurity level is called a **donor level**, and the column V impurities in Ge or Si are called donor impurities. From Fig. a and Fig. b given below, we note that the material doped with donor impurities can have a considerable concentration of electrons in the conduction band, even when the temperature is too low for the intrinsic EHP concentration to be appreciable. Thus semiconductors doped with a significant number of donor atoms will have $n_0 \gg (n_i, p_0)$ at room temperature. This is n-type material.

Atoms from column III (B, Al, Ga, and In) introduce impurity levels in Ge or Si near the valence band. These levels are empty of electrons at 0 K. Even at low temperatures, enough thermal energy is available to excite electrons from the valence band into the impurity level, leaving behind holes in the valence band. Since this type of impurity level "accepts" electrons from the valence band, it is called an *acceptor* level, and the column III impurities are acceptor impurities in Ge and Si.



Donor and acceptor atoms in the covalent bonding model of a Si crystal

Carrier Concentrations:

In calculating semiconductor electrical properties and analyzing device behavior, it is often necessary to know the number of charge carriers per cm^3 in the material. The majority carrier concentration is usually obvious in heavily doped material, since one majority carrier is obtained for each impurity atom (for the standard doping impurities). The concentration of minority carriers is not obvious, however, nor is the temperature dependence of the carrier concentrations.

To obtain equations for the carrier concentrations we must investigate the distribution of carriers over the available energy states. This type of distribution is not difficult to calculate, but the derivation requires some background in statistical methods. Since we are primarily concerned here with the application of these results to semiconductor materials and devices, we shall accept the distribution function as given.

Fermi level:

Electrons in solids obey Fermi-Dirac statistics. In the development of this type of statistics, one must consider the indistinguishability of the electrons, their wave nature, and the Pauli's exclusion principle. The rather simple result of these statistical arguments is that the distribution of electrons over a range of allowed energy levels at thermal equilibrium is

$$f(E) = \frac{1}{1 + e^{(E-E_F)/kT}}$$

k : Boltzmann's constant ($k = 8.62 \times 10^{-5} \text{ eV/K} = 1.38 \times 10^{-23} \text{ J/K}$)

kT (at 300K or 27 °C) = 25.7 meV

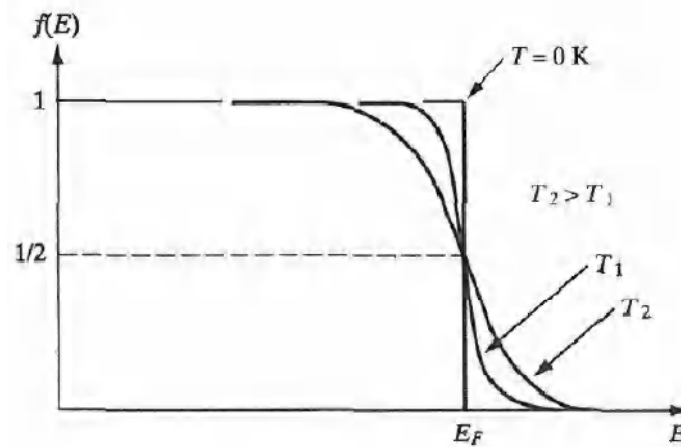
The function $f(E)$, the *Fermi-Dirac distribution function*, gives the probability that an available energy state at E will be occupied by an electron at absolute temperature T .

The quantity E_F is called the *Fermi level*, and it represents an important quantity in the analysis of semiconductor behavior.

We notice that, for an energy E equal to the Fermi level energy E_F , the occupation probability is

$$f(E_F) = \left[1 + e^{(E_F-E_F)/kT} \right]^{-1} = \frac{1}{1+1} = \frac{1}{2}$$

An energy state at the Fermi level has a probability of 1/2 (at all temperatures) of being occupied by an electron.

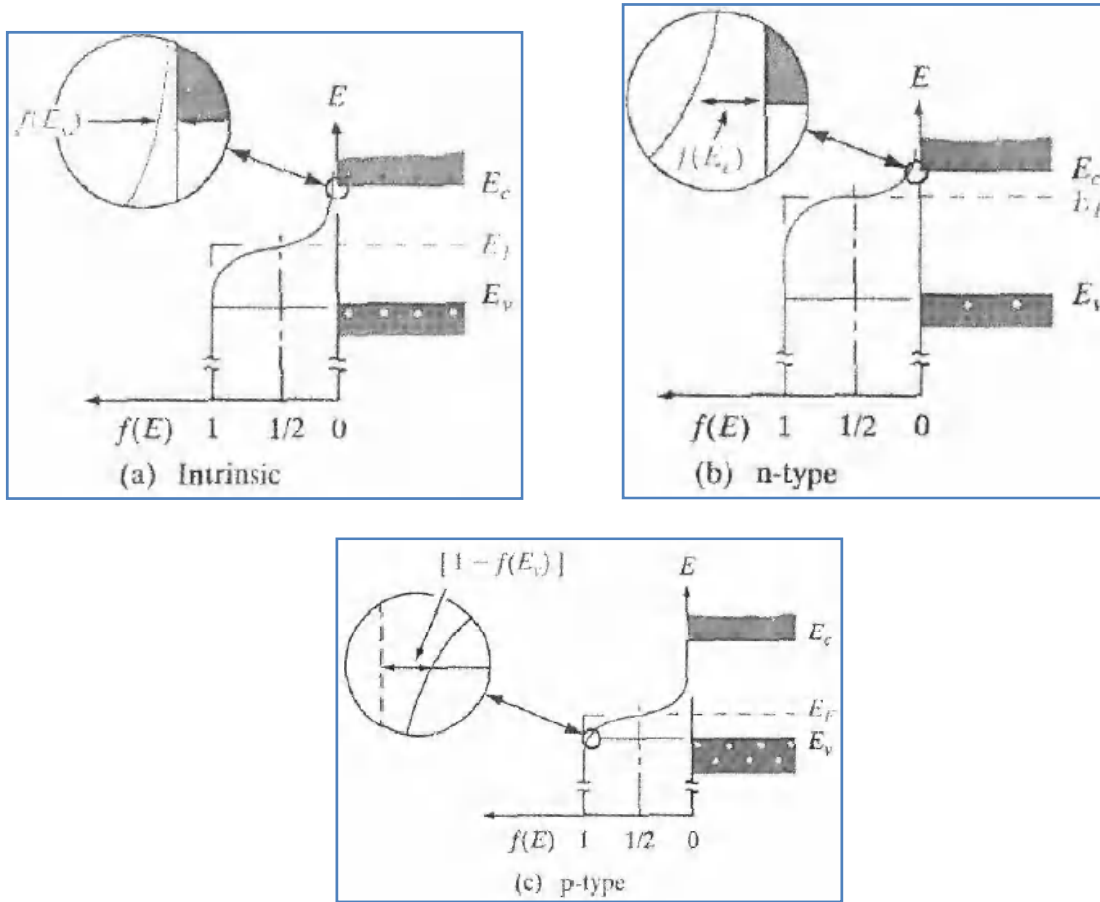


The Fermi-Dirac distribution function.

A closer examination of $f(E)$ indicates that at 0 K the distribution takes the simple rectangular form shown in Fig. With $T = 0$ in the denominator of the exponent, $f(E)$ is $1/(1 + 0) = 1$ when the exponent is negative ($E < E_F$), and is $1/(1 + \infty) = 0$ when the exponent is positive ($E > E_F$). This rectangular distribution implies that at 0 K every available energy state up to E_F is filled with electrons, and all states above E_F are empty.

The symmetry of the distribution of empty and filled states about E_F makes the Fermi level a natural reference point in calculations of electron and hole concentrations in semiconductors.

If there is no available state at E (e.g., in the band gap of a semiconductor), there is no possibility of finding an electron there. We can best visualize the relation between $f(E)$ and the band structure by turning the $f(E)$ vs. E diagram on its side so that the E scale corresponds to the energies of the band diagram.



The Fermi distribution function applied to semiconductors: (a) intrinsic material; (b) n-type material; (c) p-type material.

For intrinsic material the concentration of holes in the valence band is equal to the concentration of electrons in the conduction band. Therefore, the Fermi level E_F must lie at the middle of the band gap in intrinsic material.

Since $f(E)$ is symmetrical about E_F , the electron probability "tail" of $f(E)$ extending into the conduction band of Fig. (a) is symmetrical with the hole probability tail $[1 - f(E)]$ in the valence band. The distribution function has values within the band gap between E_V and E_C , but there are no energy states available, therefore no electron occupancy results from $f(E)$ in this range.

Actually, the probability values at E_V and E_C are quite small for intrinsic material at reasonable temperatures. For example, in Si at 300 K, $n_i = p_i = 10^{10} \text{ cm}^{-3}$, whereas the densities of available states at E_V and E_C are on the order of 10^{19} cm^{-3} . Thus the probability of occupancy $f(E)$ for an individual state in the conduction band and the hole probability $[1 - f(E)]$ for a state in the valence band are quite small.

Because of the relatively large density of states in each band, small changes in $f(E)$ can result in significant changes in carrier concentration.

In n-type material there is a high concentration of electrons in the conduction band compared with the hole concentration in the valence band. Thus in n-type material the distribution function $f(E)$ must lie above its intrinsic position on the energy scale. Since $f(E)$ retains its shape for a particular temperature, the larger concentration of electrons at E_C in n-type material implies a correspondingly smaller hole concentration at E_V . We notice that the value of $f(E)$ for each energy level in the conduction band (and therefore the total electron concentration n_0) increases as E_F moves closer to E_C . Thus the energy difference $(E_C - E_F)$ gives a measure of n ; we shall express this relation mathematically in the following section.

For p-type material the Fermi level lies near the valence band (Fig. c) such that the $[1 - f(E)]$ tail below E_V is larger than the $f(E)$ tail above E_C . The value of $(E_F - E_V)$ indicates how strongly p-type the material is.

It is usually inconvenient to draw $f(E)$ vs. E on every energy band diagram to indicate the electron and hole distributions. Therefore, it is common practice merely to indicate the position of E_F in band diagrams. This is sufficient information, since for a particular temperature the position of E_F implies the distributions in the above Fig.

Electron and Hole Concentrations at Equilibrium:

The Fermi distribution function can be used to calculate the concentrations of electrons and holes in a semiconductor, if the densities of available states in the valence and conduction bands are known. the concentration of electrons in the conduction band is

$$n_0 = \int_{E_C}^{\infty} f(E) N(E) dE$$

Where, $N(E)dE$ is the density of states (cm^{-3}) in the energy range dE .

The subscript 0 used with the electron and hole concentration symbols (n_0, p_0) indicates equilibrium conditions. The number of electrons per unit volume in the energy range dE is the product of the density of states and the probability of occupancy $f(E)$. Thus the total electron concentration is the integral over the entire conduction band. $N(E)$ is proportional to $E^{1/2}$, so the density of states in the conduction band increases with electron energy.

$$n_0 = N_C f(E_C) = \frac{N_C}{1 + e^{(E_C - E_F)/kT}} \approx N_C e^{-(E_C - E_F)/kT}$$

N_c = effective density of states located at conduction band edge

$$= 2 \left(\frac{2\pi m_n^* kT}{h^2} \right)^{3/2}$$

By similar argument, the concentration of holes in the band edge

$$p_0 = N_v [1 - f(E_v)] = N_v \left[1 - \frac{1}{1 + e^{(E_v - E_F)/kT}} \right] \approx e^{-(E_F - E_v)/kT}$$

The effective density of states in the valence band reduced to the band edge is

$$N_c = 2 \left(\frac{2\pi m_p^* kT}{h^2} \right)^{3/2}$$

For intrinsic semiconductor ($E_F = E_i$),

$$n_i = N_c e^{-(E_c - E_i)/kT} \quad \text{and} \quad p_i = N_v e^{-(E_i - E_v)/kT}$$

The product of n_0 and p_0 at equilibrium is a constant for a particular material and temperature, even if the doping is varied:

$$n_0 p_0 = N_c e^{-(E_c - E_i)/kT} N_v e^{-(E_i - E_v)/kT} = N_c N_v e^{-(E_c - E_v)/kT} = N_c N_v e^{-E_g/kT}$$

For intrinsic semiconductor

$$n_i = p_i = \sqrt{N_c N_v} e^{-E_g/2kT} \quad \text{and} \quad n_0 p_0 = n_i^2$$

The intrinsic concentration for Si at room temperature is approximately $n_i = 1.5 \times 10^{10} \text{ cm}^{-3}$.

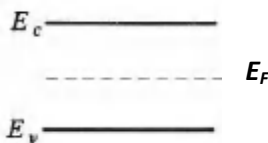
Prove that

$$n_0 = n_i e^{(E_F - E_i)/kT} \quad \text{and} \quad p_0 = p_i e^{(E_v - E_F)/kT}$$

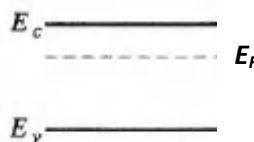
A Si sample is doped with 10^{17} As atoms/cm³. What is the equilibrium hole concentration p_0 at 300 K? Where is E_F relative to E_i ?

Ans: $E_F - E_i = 0.407 \text{ eV}$

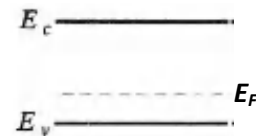
Band diagram of intrinsic and extrinsic semiconductors:



(a) Intrinsic



(b) n-type



(c) p-type