

### Physics of Semiconductor Devices Module-I

### **Introduction to Quantum Physics**

- Macro particle- Classical Physics based on Newton's laws
- Micro particle Quantum Physics; ex- electrons and high frequency electromagnetic waves
- Basic principles in quantum physics:
- (I) energy quanta :- E=hv

(II) Wave particle duality :-  $\lambda = h/p$ 

(III) Uncertainty principle :-  $\Delta x$ .  $\Delta p \ge \hbar = h/2\pi$  & other two

[ $\hbar$  = 1.054 x 10<sup>-34</sup> J-s is very small; so significant only in the subatomic level]

• Consequence: we cannot determine the exact position of an electron, but only determine the *probability* of finding an electron at a particular position

### Introduction to Quantum Physics ......

- Experimental results involving electromagnetic waves and micro particles could not be explained by classical laws of physics, hence, Schrodinger, in 1926 provided wave mechanics which incorporated the principles of quanta of Max Planck, the wave-particle duality of de Broglie & uncertainty principle.
- > Motion of electrons in a crystal is explained by wave theory.
- > Wave theory is described by Schrodinger's wave equation in wave function  $\psi$ ,

$$\sum_{n=1}^{\infty} \frac{-\hbar^2}{2m} \cdot \frac{\partial^2 \Psi(x,t)}{\partial x^2} + V(x)\Psi(x,t) = j\hbar \frac{\partial \Psi(x,t)}{\partial t}$$
 time-dependent

& 
$$\frac{\partial^2 \psi(x)}{\partial x^2} + \frac{2m}{\hbar^2} (E - V(x))\psi(x) = 0$$
 time-independent

 $\psi_{\text{r}}$  is used to describe the behavior of the particle with wave nature & is a complex quantity

#### Introduction to Quantum Physics ......

• Probability density given by

$$|\Psi(x,t)|^2 = \Psi(x,t)\cdot \Psi^*(x,t)$$

 $= |\psi(x)|^2$ 

With 
$$\int_{-\infty}^{\infty} |\psi(x)|^2 dx = 1$$

Boundary conditions used for solution of the Sch. Eqn.

 $\psi(x)$  must be finite, single-valued, and continuous.  $\partial \psi(x)/\partial x$  must be finite, single-valued, and continuous.

#### Introduction to Quantum Physics ......

#### • Application of Sch. Eqn.

Free Particle: continuous energy  $E = \frac{\hbar^2 k^2}{2m}$ Particle in Potential Well : energy is quantized and discrete  $E_n = \frac{\hbar^2 n^2 \pi^2}{2ma^2}$ Particle in Potential step: finite probability of particle moving to step region when E < V<sub>0</sub>

- Particle in Potential barrier: Tunneling
- **•** Wave theory may be extended to the ator  $E_{n} = \frac{-m_{0}e^{4}}{(4\pi\epsilon_{0})^{2}2\hbar^{2}n^{2}}$  **•** With  $n = 1, 2, 3, \dots$ quantum  $l = n 1, n 2, n 3, \dots, 0$ numbers  $|m| = l, l 1, \dots, 0$   $\psi_{100} = \frac{1}{\sqrt{\pi}} \cdot \left(\frac{1}{a_{0}}\right)^{3/2} e^{-r/a_{0}}$   $a_{0} = \frac{4\pi\epsilon_{0}\hbar^{2}}{m_{0}^{2}} = 0.529 \text{ Å}$

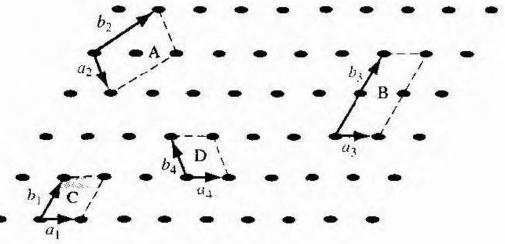
Electron distribution in the atom obey Pauli's exclusion principle

### Introduction to Quantum theory of solids

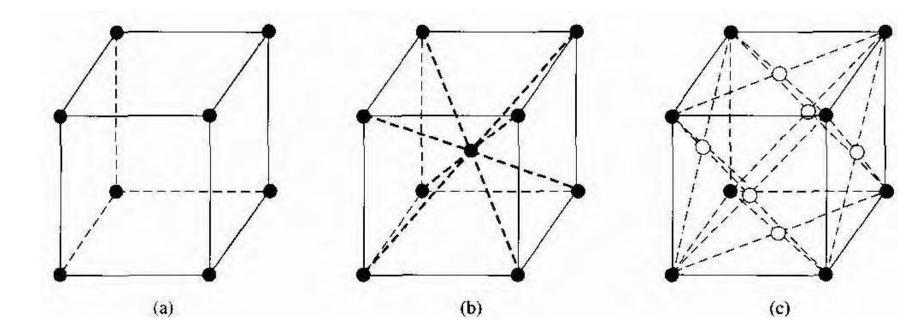
- Crystal = lattice + basis
- Basis has atoms in it, which have bound electron as well as free electrons in them. The free electrons inside the crystalline solid roam freely and are mainly

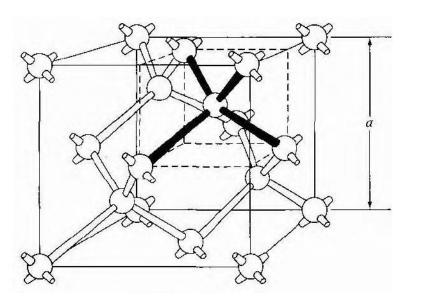
responsible for

conduction phenomena



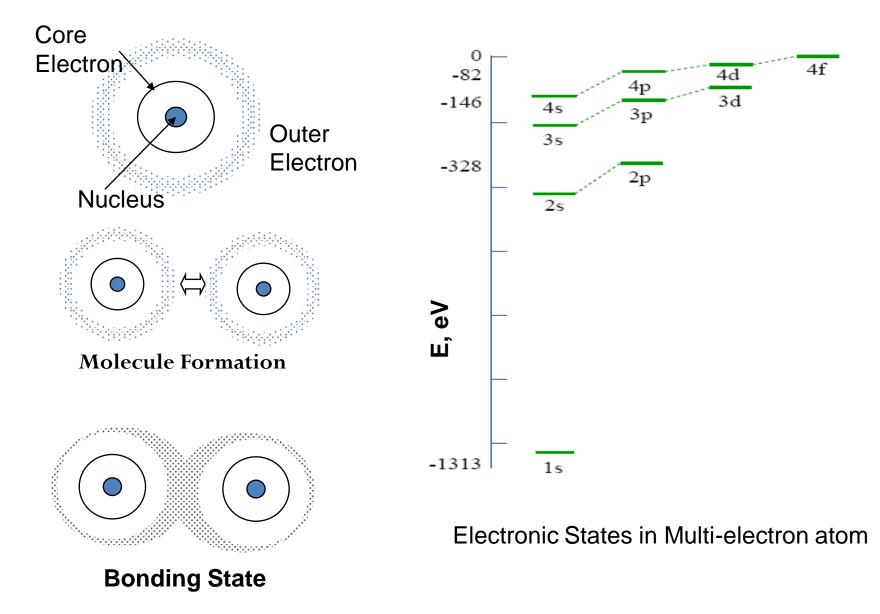
 Inside the crystal structure the positive ions are submerged in the sea of free electrons





### Introduction to Quantum theory of solids.....

- Electrons inside the atoms of a solid have wave nature
- Free electrons move throughout the crystal, but restricted within the surfaces; hence are treated as particle trapped in a box and studied with help of Sch. Eqn.
- Electrons in a solid can take up discrete energy values & obey Pauli's principle for their distribution
- To determine the electrical properties in a semiconductor crystal and develop the current-voltage characteristic for device application, it is important to understand the properties of the electrons in the crystal lattice and the statistical characteristics of the large no of electrons in the crystal.
- Behavior of free electron is different from electron in the potential field of the crystal
- As current is due to flow of charge, electron behavior in external electric field is important



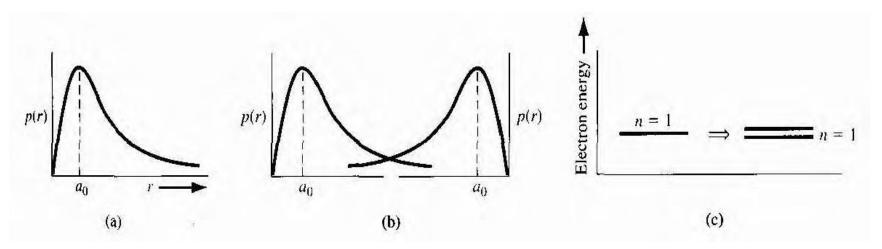
# Energy Bands Consider: Atom 'M' with single outer 's' electron n=1 n=2 $M_2$ $M_2$

• The allowed energy levels for an atom are discrete (2 electrons with opposite spin can occupy a state)

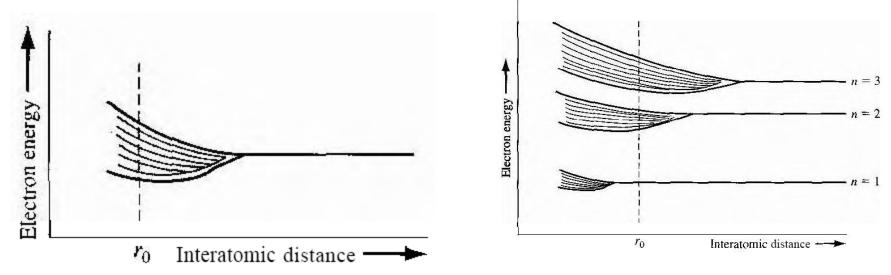
**Electron Energy** 

- When atoms are brought into close contact, these energy levels split
- If there are a large number of atoms, the discrete energy levels form a "continuous" band
- As gas condenses into a solid, one single energy state of an atom expands into a band with closely spaced energy states. This also leads to lowering of total energy.
- As the two atoms get closer than 'a', repulsion due to core electrons/nuclei increases.

### Energy bands in solid (Qualitative)



since no two electrons can have the same quantum number, the discrete energy must split into a band of energies in order that each electron can occupy a distinct quantum state.



### **Energy bands in solid: Kronig-Penny model**

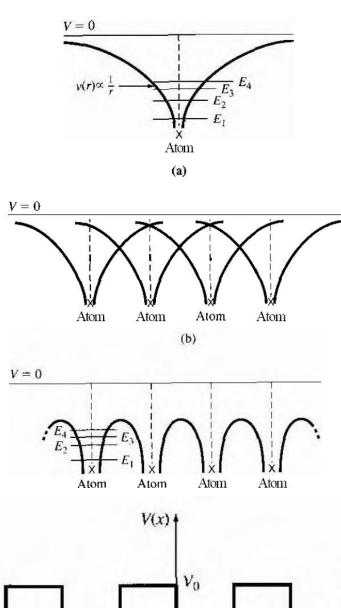
 Actually the electron sees a periodic potential inside a solid with spatial period of 'a' due to its crystal structure. The periodic potential can be approximated by the Kronig Penny model which is theoretically solvable.

$$V(x) = V(x + na)$$

Time independant Schrödinger's equation :

 $\frac{d^2\psi}{dx^2} + \frac{2m_e}{\hbar^2} \mathbf{I} - \mathbf{V}(\mathbf{x})\mathbf{y} = \mathbf{0} \text{ inside the periodic lattice.}$ 

Solution : 
$$\psi(x) = u_k(x)e^{\pm ikx} \iff Bloch$$
 function  
where  $u_k(x) = u_k(x + a) \iff A$  periodic function of x



II

0

II

-(a+b)

I

-b

I

II

a

I

(a+b)

H

x.

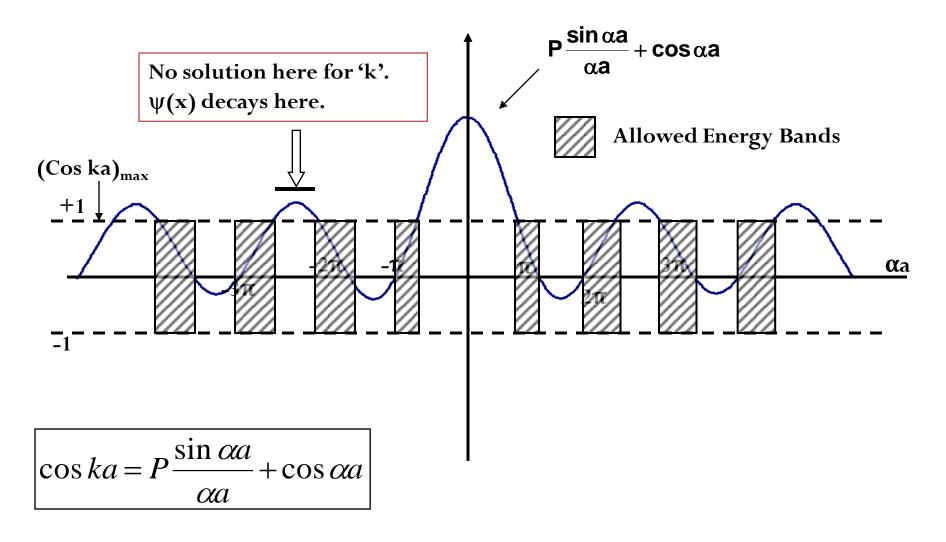
Solution for Shrödinger's equation for Kronig Penny model is possible for energies that satisfy the following conditions

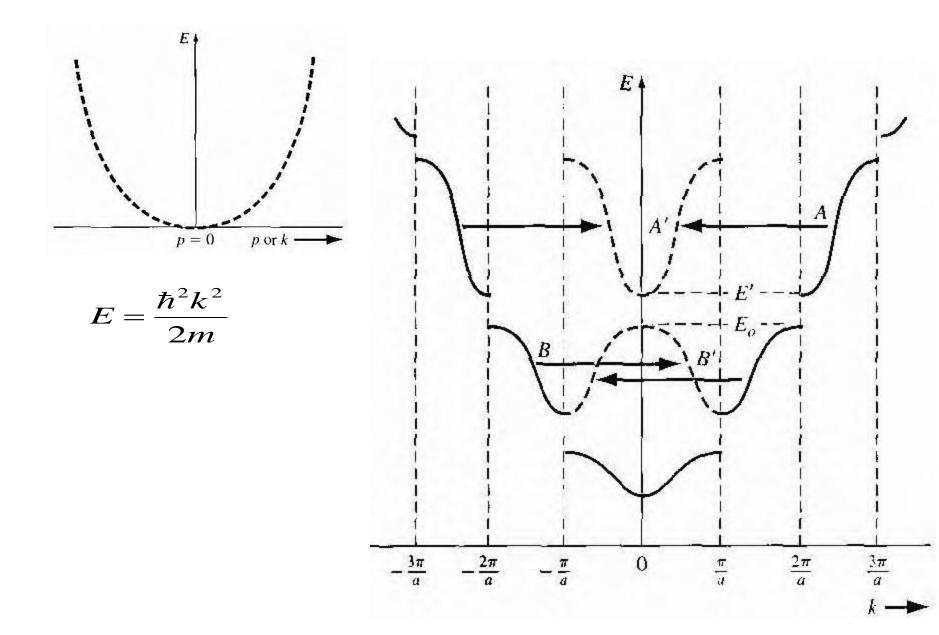
$$\cos ka = P \frac{\sin \alpha a}{\alpha a} + \cos \alpha a$$

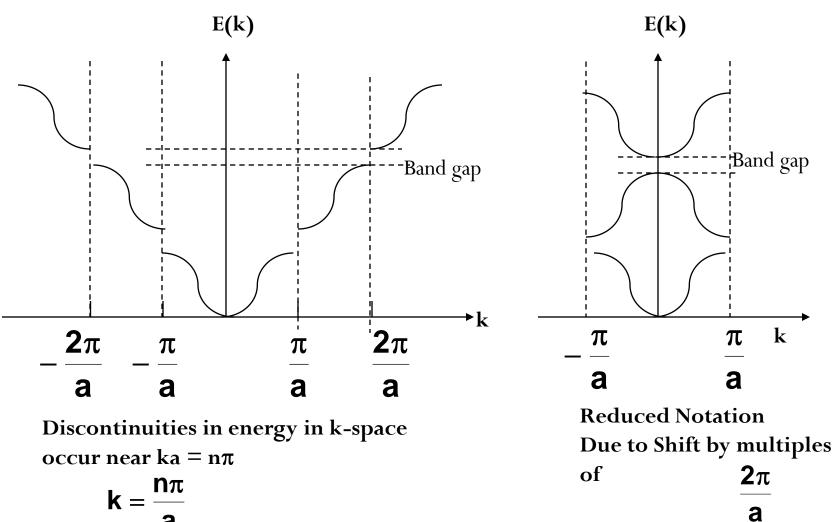
where 
$$P = \frac{m_e a}{\hbar^2} V_0 w$$
 &  $\alpha = \frac{\sqrt{2m_e E}}{\hbar}$ 

Since -1 < cos ka < +1, no solution is possible, if RHS of equation is less than one or greater than one.

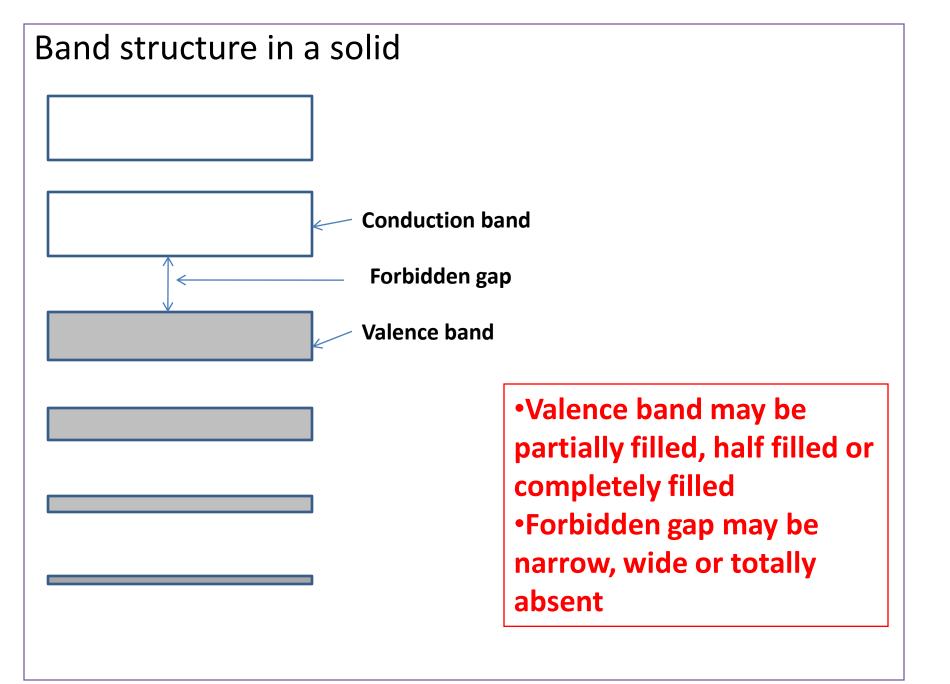
#### **Kronig Penny model:**

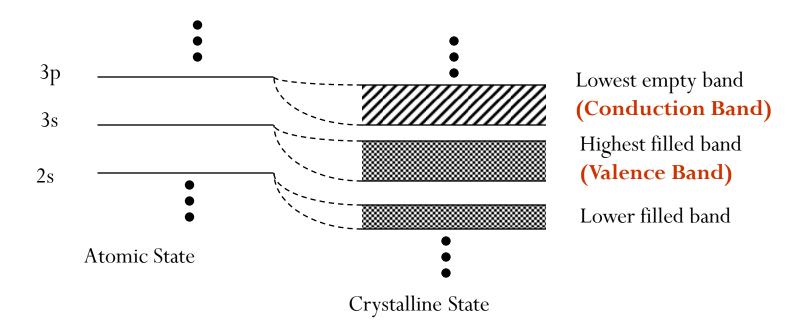




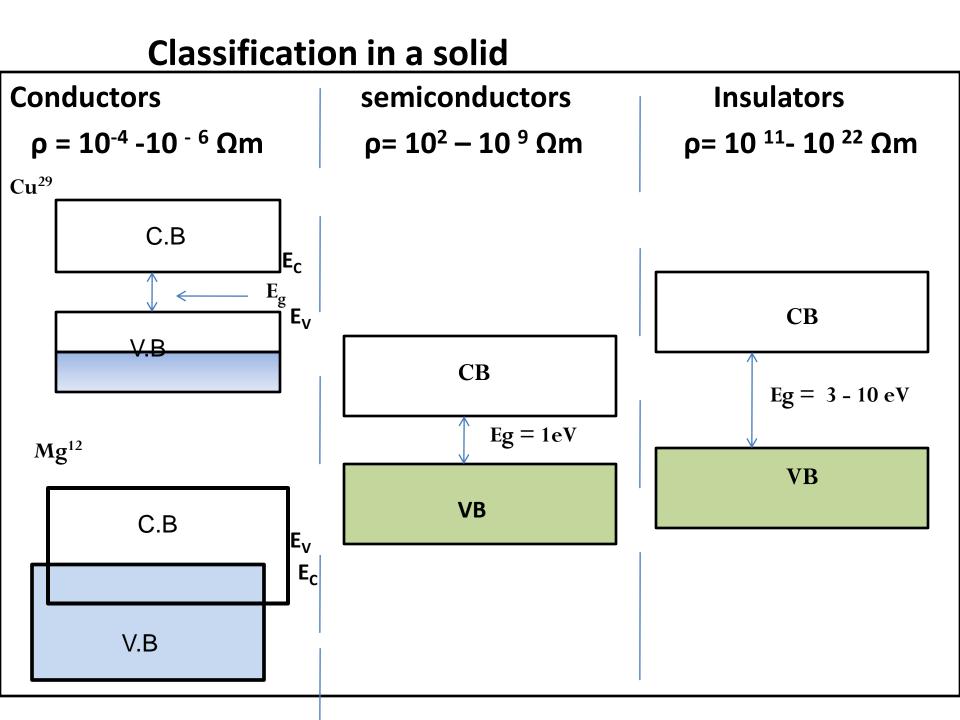


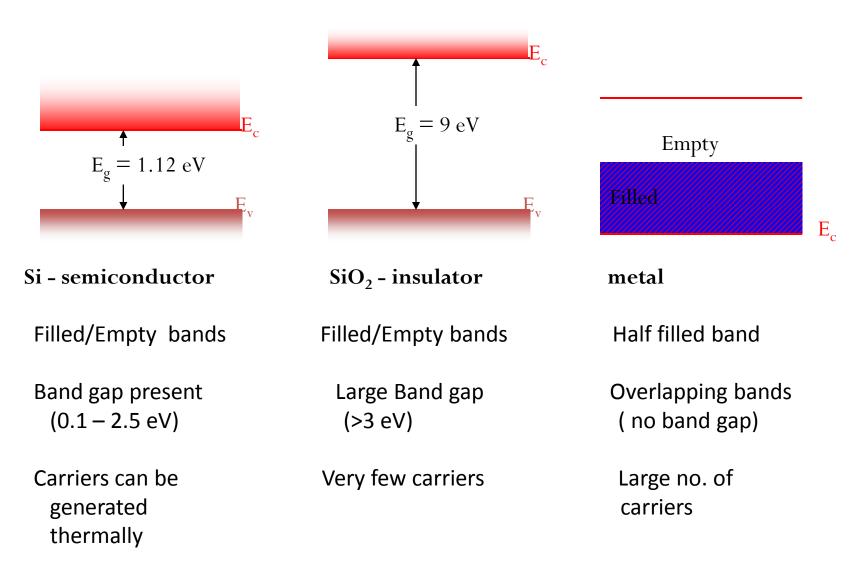
a

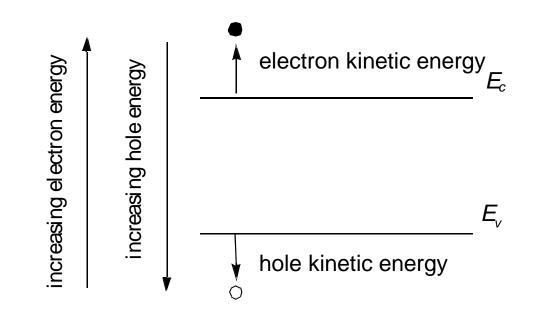




- Energy states of atom expand into energy bands of a crystal.
- The lower bands are filled and higher bands are empty in a semiconductor.
- The highest filled band is the valence band.
- The lowest empty band is the conduction band .

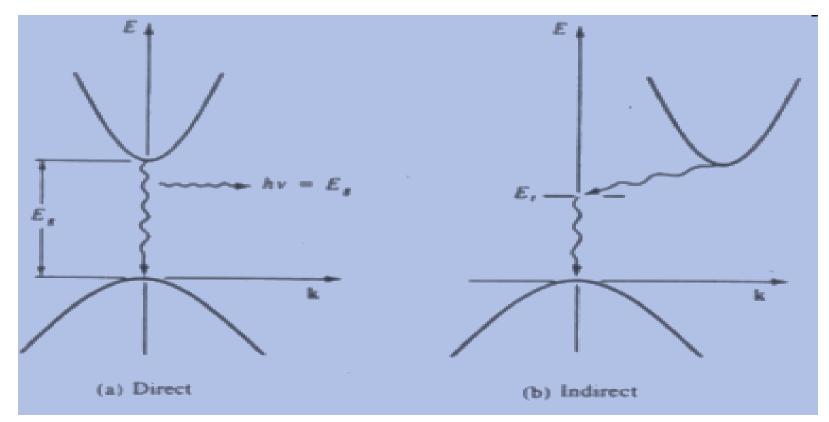






- Both electrons and holes tend to seek their lowest energy positions.
- Electrons tend to fall in the energy band diagram.
- Holes float up like bubbles in water

The extrema for the conduction and valence bands are at different values of K for silicon and germanium --these are called *indirect* bandgap semiconductors The conduction band minimum and valence band maximum both occur at K=0 for GaAs --this is called a *direct* bandgap semiconductor.

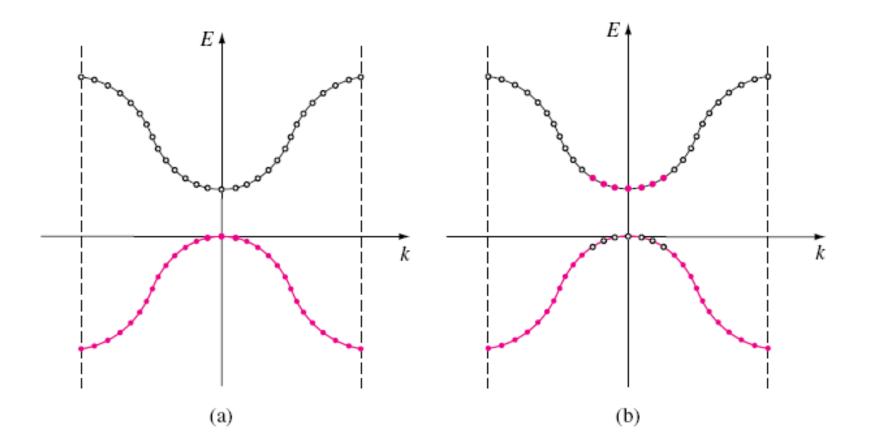


Direct band gap Ex: GaAs indirect bandgap:  $\Delta K$  is large but for a direct bandgap:  $\Delta K=0$  and *light* in direct bandgap materials (GaAs, GaN, etc) but *heat* in indirect bandgap materials (Si, Ge)

Indirect band gap Ex: Si,Ge

### **Electrons and Holes**

- Holes are the electron voids in the valence band.
- Electrons and holes carry negative and positive charge (±q) respectively.
- higher position in the energy band diagram represents a higher electron energy. The minimum conduction electron energy is Ec. Any energy above Ec is the electron kinetic energy. Electrons may gain energy by getting accelerated in an electric field and may lose energy through collisions with imperfections in the crystal.
- A lower location in the energy diagram represents a higher hole energy It requires energy to move a hole "downward" as it is equivalent to moving an electron upward. Ev is the minimum hole energy.
- The forbidden gap=  $E_c E_v = E_g$



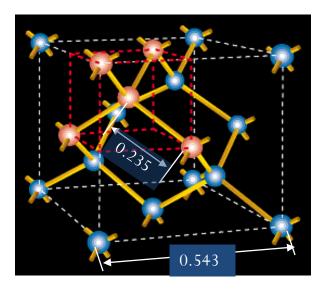
E versus k diagram of the conduction and valence bands of a (a) T = 0 K and (b) T > 0 K.

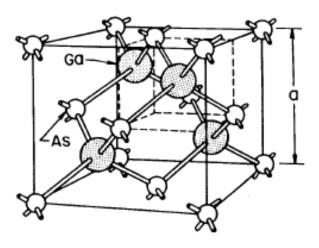
### **Semiconductor Silicon**

### Why Silicon Technology is so dominant?

- Band gap is ~1 eV.
- Single element semiconductor
- Almost perfect material available purity and crystalline perfection
- Easy processability
- Silicon silicon oxide interface almost perfect
- Amazing chemical, physical and electronic properties
- Silicon second most abundant element after oxygen

### **Semiconductor Silicon**







#### Silicon :

- Diamond cubic lattice: atoms tetrahedrally bonded (valence electronic shared no free electrons)
- 4 nearest neighbours
- Lattice parameter : 0.543 nm
- Atomic spacing : 0.235 nm
- 8 atoms per unit cells
- Si atomic density : 5x10<sup>28</sup> at/m<sup>3</sup>

### **Semiconductor Silicon**

#### Silicon Bond Model:

Si is in Column IV of the periodic table

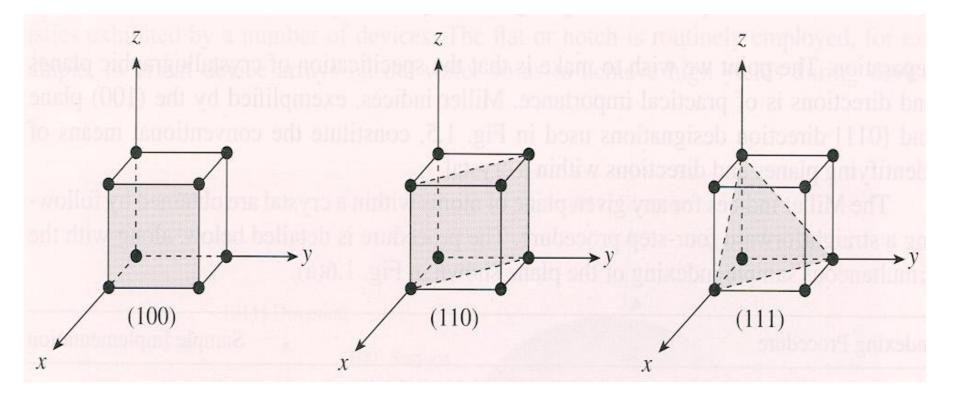
#### **Electonic structure of Si atom:**

- 10 core electrons 1s<sup>2</sup> 2s<sup>2</sup>p<sup>6</sup>
- 4 valence electrons 3s<sup>2</sup>p<sup>2</sup>
- 3s and 3p orbitals hybridize to form 4 tetrahedral 3sp orbitals
- Each orbital has one electron and is capable forming one covalent bond with a neighbouring atom
- Covalent bonds

#### **Other Semiconductors**:

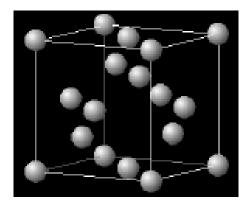
Ge, C, Si<sub>1-x</sub> Ge<sub>x</sub>
GaAs, InP, InGaAs, ZnSe, CdTe
On an average, 4 valence electrons per atom.

	IIIA	IVA	VA	VIA
	B	0 °	N	0
IIB	Al	Si	P	S
Zn	Ga	Ge	As	34 Se
Cd	۱n	Sn	Sb	Te



# Silicon Crystal

Unit cell:

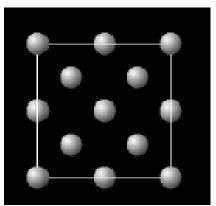


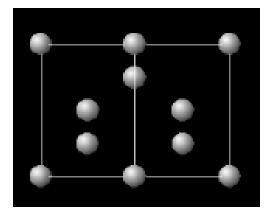
Si lattice constant =

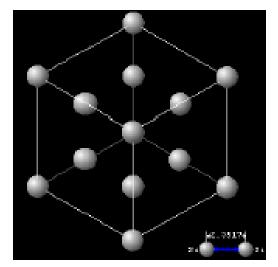
0.5431 nm

 $\rightarrow$  5 X 10<sup>28</sup> at/m<sup>3</sup>

View in <100> direction View in <110> direction View in <111> direction



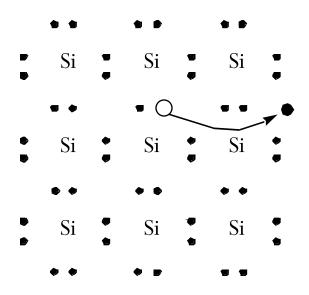


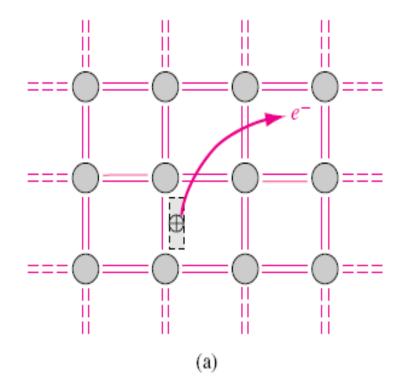


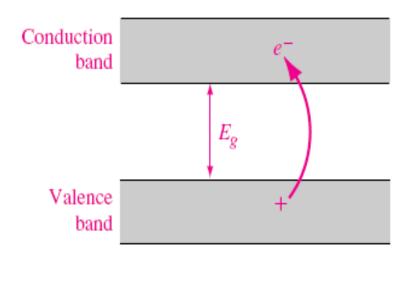
http://jas.eng.buffalo.edu/education/solid/unitCell/home.html

### **Intrinsic Semiconductor (Si)**

- At OK, there are no free electrons.
- At finite temperature, some electrons break free due to thermal excitation energy, k<sub>B</sub>T and a conduction electron and hole are created.
- A hole is absence of electron and has positive charge equal in magnitude to electronic charge.
- The electrons and holes are not localised as shown in the picture, but form a cloud as per quantum physics.







(b)

### **Effective mass**

An electron in crystal may behave as if it had a mass different from the free electron mass  $m_0$ . There are crystals in which the effective mass of the carriers is much larger or much smaller than  $m_0$ . The effective mass may be anisotropic, and it may even be negative. The important point is that the electron in a periodic potential is accelerated relative to the lattice in an applied electric or magnetic field as if its mass is equal to an effective mass.

In addition to an externally applied force, there are internal forces in the crystal due to positively charged ions or protons and negatively charged electrons, which will influence the motion of electrons in the lattice

$$F_{\text{total}} = F_{\text{ext}} + F_{\text{int}} = ma$$

it is difficult to take into account all of the internal forces, so we write

$$F_{\text{ext}} = m^* a$$

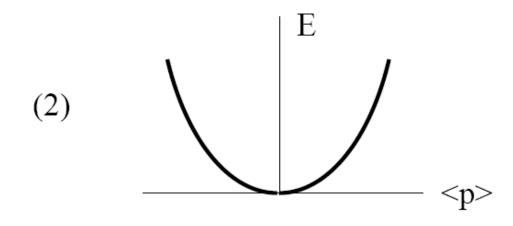
*m\**, called the *effective mass*, takes into account the particle mass and also the effect of the internal forces, it is related to the *E* versus *k* curves

### Effective Mass ......

If the electron is free then E represents the kinetic energy only. It is related to the wave vector k and momentum p by

(1) 
$$E = \frac{\hbar^2 k^2}{2m_0} = \frac{p^2}{2m_0}$$

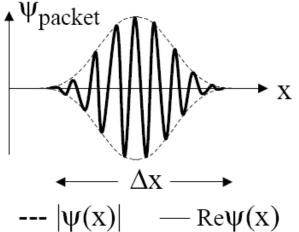
Therefore, the quantum mechanical and classical free particles exhibit precisely the same energy-momentum relationship, as shown below.



#### Effective Mass ......

The velocity of the real particle is the phase velocity of the wave packet envelope. It is called the group velocity and its relation to energy and momentum is obtained from (1)

(3) 
$$v_g = \frac{dE}{dp} = \frac{1}{\hbar} \frac{dE}{dk}$$



Here, E and k are interpreted as the center values of energy and crystal momentum, respectively.

Now, what happens when an "external" force F acts on the wavepacket? F could be any force other than the crystalline force associated with the periodic potential. The crystalline force is already taken into account in the wavefunction solution.

#### **Effective Mass .....**

The work done by the force on the wavepacket will then be

(4) 
$$dE = Fdx = Fv_g dt$$

From that we get the force expression using (3)

(5) 
$$F = \frac{1}{v_g} \frac{dE}{dt} = \frac{1}{v_g} \frac{dE}{dk} \frac{dk}{dt}$$
  
(6) 
$$F = \frac{d(\hbar k)}{dt}$$

The acceleration is found taking time derivative of (3)

(7) 
$$a = \frac{dv_g}{dt} = \frac{1}{\hbar} \frac{d}{dt} \left(\frac{dE}{dk}\right) = \frac{1}{\hbar^2} \left(\frac{d^2E}{dk^2}\right) \frac{d(\hbar k)}{dt}$$

#### **Effective Mass .....**

Finally, we obtain the effective mass equation

(8) 
$$F = m * \cdot \frac{dv_g}{dt}$$
  
(9) 
$$m * = \frac{1}{\frac{1}{\hbar^2} \frac{d^2 E}{dk^2}}$$

The equation (8) is identical to Newton's second law of motion except that the actual particle mass is replaced by an *effective* mass  $m^*$ .

effective mass is a parameter that relates the quantum mechanical results to the classical force equations, provided that the internal forces and quantum mechanical properties are taken into account through the effective mass

The motion of the free electron is in the opposite direction to the applied electric field because of the negative charge, as a = -q E /m

Different lattice spacing lead to different curvatures for E(K) and <u>effective</u> <u>masses</u> that depend on the direction of motion.

# Effective Mass ......

### Effective mass of electrons and holes:

So m<sup>\*</sup> =  $\hbar^2 \left( \frac{\partial^2 E}{\partial k^2} \right)^{-1} \propto$  curvature of the band

Since, the second derivative at a minima is positive, electrons at the bottom of conduction band has negative charge and positive mass (larger  $d^2E/dK^2$ ; light m<sup>\*</sup>)

**E(k)** m<sub>2</sub>

 $m_{2} > m_{4}$ 

Again, second derivative at a maxima is negative, the effective mass will be negative. But, a = -q E / -m = q E / mparticle at the top of valence band move in the field direction; these are called holes, has a positive effective mass and a positive electronic charge smaller  $d^2E/dK^2$ ; heavy m<sup>\*</sup>

	Ge	Si	GaAs
E <sub>g</sub> , eV (300K)	0.66	1.12	1.42
m <sub>n</sub> /m <sub>o</sub>	0.55	1.08	0.067
m <sub>p</sub> /m <sub>o</sub>	0.37	0.56	0.48

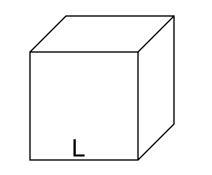
 $m_0 = \text{rest mass of electron} = 9.11 \text{ x } 10^{-31} \text{ kg}$ 

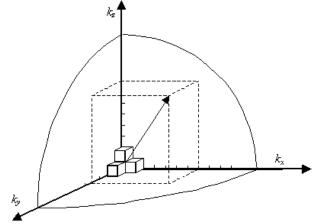
# **Density of states**

- The number of carriers contribute to the conduction process is a function of the number of available energy or quantum states. Each state represents a unique spin (up and down) and unique solution to the Schrodinger's wave equation for the periodic electric potential function.
- Electrons are fermions or Fermi particles, which obey Pauli's exclusion principle so each quantum state can hold either one electron or none.
- If N is the total no. of electrons, in 3D, electrons will occupy a sphere of radius k, then highest occupied state n<sub>f</sub> = N/2
- Allowed energy bands are made up of discrete energy levels. If the number of states in a small range of energy  $\Delta E$  per volume in the band is counted, it is called **density of states**.

# **Density of States**

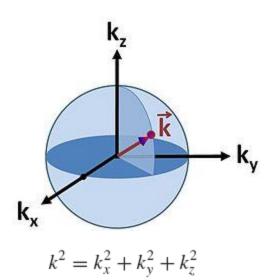
Consider free electrons inside a metal of cubic shape and size 'L'.

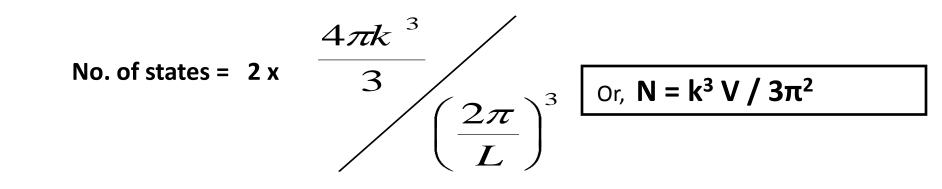




$$\Delta p \Delta x = h, \quad \Delta x = L \quad \& \quad \Delta p = \hbar k$$
  
So, 
$$\Delta k = \frac{2\pi}{L} = \text{size of each state in } k - \text{space}$$
  
Volume of each state =  $\left(\frac{2\pi}{L}\right)^3$   
Volume of sphere in k-space =  $\frac{4}{3}\pi k^3$ 

Volume of sphere in k-space =





#### **Density of state**

g(E) = Number of energy states per unit energy range per unit volume $= \frac{1}{V} \frac{dN}{dE}$ 

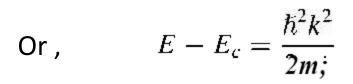
$$= \frac{1}{V} \frac{d}{dE} \left( \frac{k^{3}V}{3\pi^{2}} \right) \qquad \text{as, } E = \hbar^{2} k^{2} / 2m \text{ or } k = (2mE/\hbar^{2})^{1/2}$$
$$= \frac{d}{dE} \left[ \frac{1}{3\pi^{2}} \left( \frac{2mE}{\hbar^{2}} \right)^{\frac{3}{2}} \right] \qquad = \frac{1}{2\pi^{2}} \left( \frac{2m}{\hbar^{2}} \right)^{\frac{3}{2}} E^{\frac{1}{2}}$$

# **Density of states in semiconductors**



$$\frac{4\pi (2m)^{3/2}}{h^3}\sqrt{E}$$

For a <u>semiconductor</u>, approximating the E vs k curve to a parabola at the bottom of the conduction band for electrons, we have



 $E = E_c + \frac{\hbar^2 k^2}{2m_n^*}$ 

DOS in conduction band = 
$$g_c(E) = \frac{4\pi (2m_n^*)^{3/2}}{h^3} \sqrt{E - E_c}$$

Which is valid for Valid for all  $E \ge E_c$ 

 $\frac{\pi}{-\frac{\pi}{a}} \qquad \frac{\pi}{a} \qquad \frac{\pi}{a}$ C.B & V.B in reduced k-space

**E(k)** 

DOS  $\propto \sqrt{E}$ 

 $E = p^2/2m$ 

# **Density of states.....**

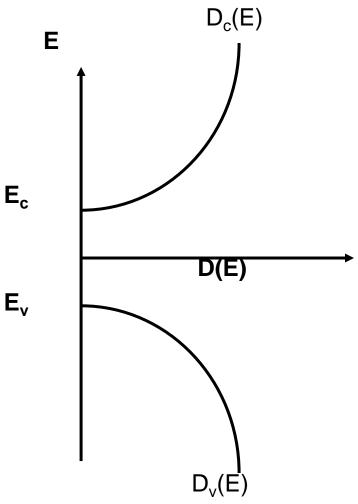
• Similarly, approximating at the top of the valence band for the holes,

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

• Or, 
$$E_v - E = \frac{\hbar^2 k^2}{2m_p^*}$$

• =g<sub>v</sub>(E)= 
$$\frac{4\pi (2m_p^*)^{3/2}}{h^3} \sqrt{E_v - E}$$

Which is valid for all  $E \le E_v$ 

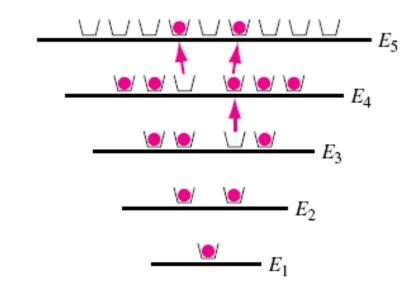


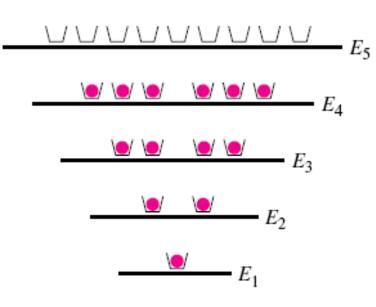
# Fermi-level and Fermi-Dirac distribution

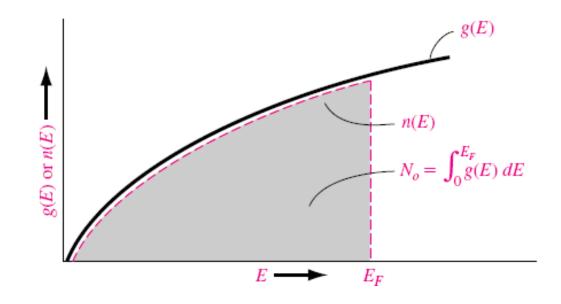
- At T = OK, all the possible quantum energy state would be filled up with two electrons each up to a maximum level called the Fermi Level. The energy of the state at the Fermi level is known as the Fermi energy, E<sub>F</sub>.
- Density of states tells us how many states exist at a given energy E. The Fermi function f(E) specifies how many of the existing states at the energy E will be filled with electrons. The function f(E) specifies, under equilibrium conditions, the probability that an available state at an energy E will be occupied by an electron. It is a probability distribution function.
- Both electron and hole are Fermi-Dirac particles with spin ½.

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

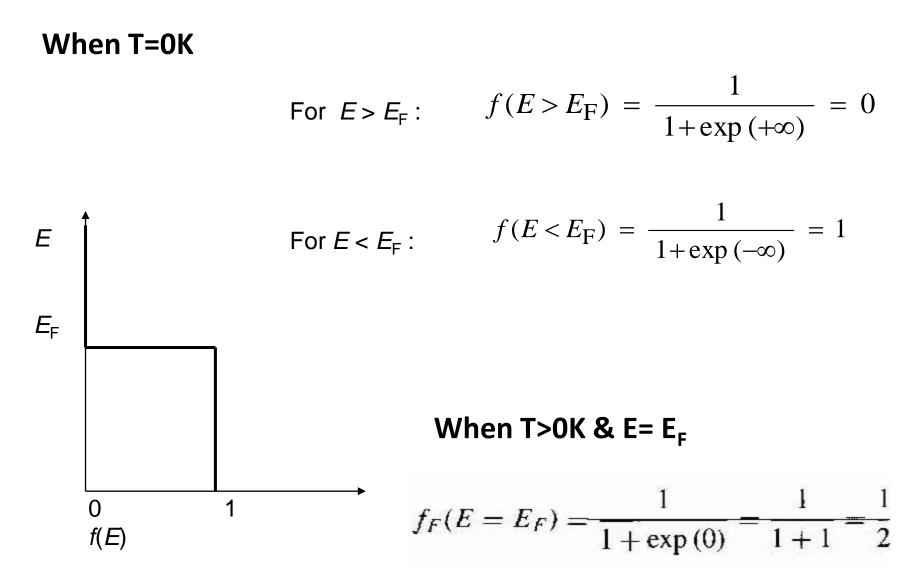
k = Boltzmann constant =  $1.38 \times 10^{-23}$  J/K =  $8.6 \times 10^{-5}$  eV/K



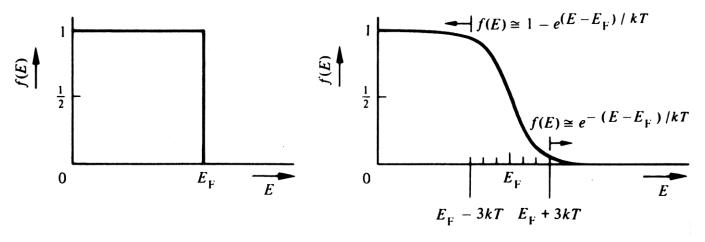




## **Fermi-Dirac distribution**

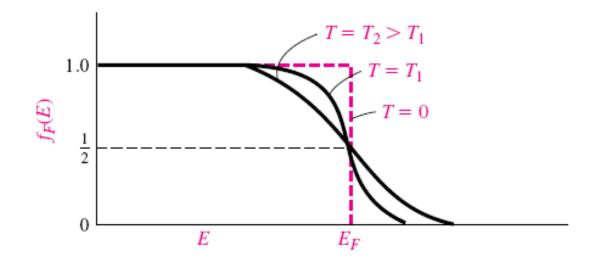


#### **Temperature dependence of Fermi-Dirac distribution Function**

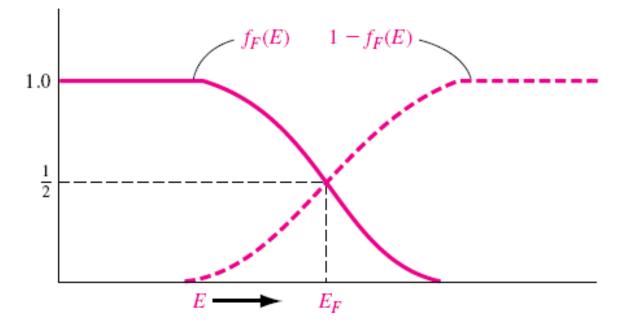


(a) *T* → 0 K

(b) T > 0 K



The probability of a state a distance dE above  $E_F$  being occupied is the same as the probability of a state a distance dE below  $E_F$  being empty. The function  $f_F$  (E) is symmetrical with the function  $1 - f_F$  (E) about the Fermi energy,  $E_F$ .

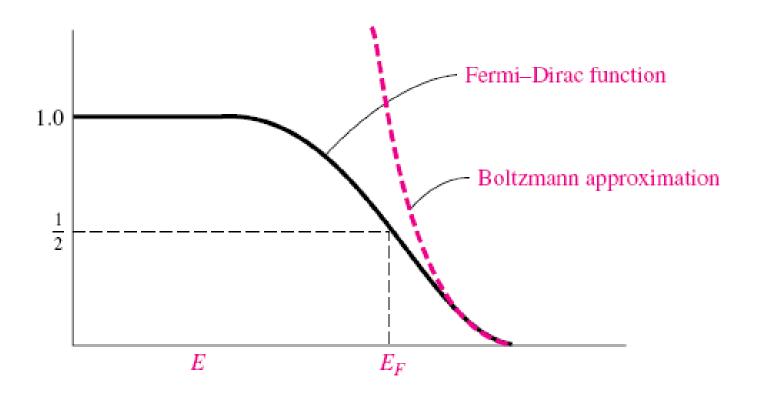


The probability of a state being occupied,  $f_F(E)$ , and the probability of a state being empty,  $1 - f_F(E)$ .

when  $E - E_F >> kT$ , the exponential term in the denominator is much greater than unity. We may neglect the 1 in the denominator, so the Fermi–Dirac distribution function becomes

$$f_F(E) \approx \exp\left[\frac{-(E-E_F)}{kT}\right]$$

is known as the Maxwell–Boltzmann approximation, or Boltzmann approx.



# SEMICONDUCTOR IN EQUILIBRIUM

- Equilibrium implies that no external forces (voltages, electric fields. Magnetic fields or temperature gradients) are acting on the semiconductor. All properties of the semiconductor will be independent of time in this case.
- Equilibrium result will be extended to the case when a voltage is applied to a semiconductor device.
- Initially an intrinsic semiconductor is considered.
- Current in a semiconductor is determined by the number of electrons in the conduction band and the number of holes in the valence band
- Both of them can be calculated from the density of states function and the Fermi distribution function

# **Equilibrium Carrier concentration**

 Distribution of electrons in the conduction band is given by the density of allowed quantum states times the probability that a state is occupied by an electron

• 
$$n(E) = g_c(E) f_F(E)$$

• Total electron concentration per unit volume in the conduction band at thermal equilibrium

• 
$$n_0 = \int g_c(E) f_F(E) dE$$

- For the holes in the valence band,
- $p(E) = g_v(E)[1 f_F(E)]$
- Equilibrium concentration of holes in the valence band

$$p_0 = \int g_v(E) [1 - f_F(E)] dE$$

- Assuming that Fermi level is midway in the band gap, for electron in the conduction band, E > E<sub>f</sub>
- If  $E_c E_f > kT$  then  $E-E_f > kT$ ; so F-D function reduces to Boltzmann fn.

$$f_F(E) = \frac{1}{1 + \exp \frac{(E - E_F)}{kT}} \approx \exp \frac{\left[-(E - E_F)\right]}{kT}$$

• Thermal eqbm. Electron density in the conduction band

$$n_0 = \int_{E_c}^{\infty} \frac{4\pi (2m_n^*)^{\frac{3}{2}}}{h^3} \sqrt{(E - E_c)} \exp[\frac{-(E - E_F)}{kT}] dE$$

• Let, 
$$x = \frac{E - E_c}{kT}$$

• So in the integral,

$$n_0 = \frac{4\pi (2m_n^* kT)^{\frac{3}{2}}}{h^3} \exp\left[\frac{-(E - E_F)}{kT}\right]_0^\infty x^{\frac{1}{2}} \exp(-x) dx$$

The integral is a gamma function whose value is =

Then, 
$$n_0 = 2 \left[ \frac{2\pi m_n^* k_B T}{h^2} \right]^{\frac{3}{2}} e^{-\frac{(E_c - E_f)}{k_B T}} = N_c e^{-\frac{(E_c - E_f)}{k_B T}}$$

where 
$$N_c = 2\left[\frac{2\pi m_n^* k_B T}{h^2}\right]^{\frac{3}{2}} = 2.8 \times 10^{19} / cm^3$$
 for Si at 300K

 $\frac{1}{2}\sqrt{\pi}$ 

Similarily

$$p_{0} = N_{v}e^{-\frac{(E_{f} - E_{v})}{k_{B}T}}$$
  
where  $N_{v} = 2\left[\frac{2\pi m_{p}^{*}k_{B}T}{h^{2}}\right]^{\frac{3}{2}} = 1.04x10^{19} / cm^{3}$  for Si at 300K

# $N_c$ and $N_v$ are effective density of states at the bottom of conduction and the top of valence bands respectively.

	$N_c~(\mathrm{cm}^{-3})$	$N_v ({ m cm}^{-3})$	$m_n^*/m_0$	$m_p^*/m_0$
Silicon	$2.8 \ge 10^{19}$	$1.04 \times 10^{19}$	1.08	0.56
Gallium arsenide	$4.7 \times 10^{17}$	$7.0 \times 10^{18}$	0.067	0.48
Germanium	$1.04 \times 10^{19}$	$6.0 \times 10^{18}$	0.55	0.37

Table 4.1 | Effectivedensity of states function and effective mass values

#### **Intrinsic Carrier Concentration:**

In the intrinsic semiconductor the concentration of electrons in the conduction band and concentration of holes in the valence band are same.

#### n<sub>i</sub>= p<sub>i</sub>

The fermi energy level is called intrinsic fermi energy level  $\mathbf{E}_{fi}$ 

So 
$$\mathbf{n_0} = \mathbf{n_i}$$
 and  $\mathbf{p_0} = \mathbf{p_i}$ 

$$n_{i}p_{i} = N_{c}N_{v}e^{-\frac{E_{c}-E_{v}}{k_{B}T}} = N_{c}N_{v}e^{-\frac{E_{g}}{k_{B}T}} = n_{i}^{2}$$

For intrinsic semiconductor,  $n = p = n_i = \sqrt{N_c N_v} e^{-\frac{E_g}{2k_B T}}$ 

n<sub>i</sub> = intrinsic carrier concentration

$$= 3.9 \times 10^{22} \, \mathrm{T}^{\frac{3}{2}} \mathrm{e}^{-\frac{\mathrm{E}_{\mathrm{g}}}{2\mathrm{k}_{\mathrm{B}}\mathrm{T}}}$$

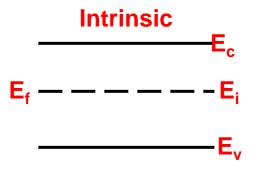
Value of n<sub>i</sub> at 300K

Silicon	$n_t = 1.5 \times 10^{10} \mathrm{cm}^{-3}$
Gallium arsenide	$n_{\rm r} = 1.8 \times 10^6  {\rm cm}^{-3}$
Germanium	$n_{\rm r} = 2.4 \text{ x } 10^{13} \text{ cm}^{-3}$

### **Intrinsic Fermi Level:**

As 
$$\mathbf{n_i} = \mathbf{p_i} \implies N_c e^{-\frac{E_c - E_f}{k_B T}} = N_v e^{-\frac{E_f - E_v}{k_B T}}$$

Taking 
$$\log_{e}$$
,  $\ln N_{c} - \frac{E_{c} - E_{f}}{k_{B}T} = \ln N_{v} - \frac{E_{f} - E_{v}}{k_{B}T}$   
So,  $E_{f} = \frac{E_{c} + E_{v}}{2} + \frac{k_{B}T}{2} \ln \left(\frac{N_{v}}{N_{c}}\right)$ 

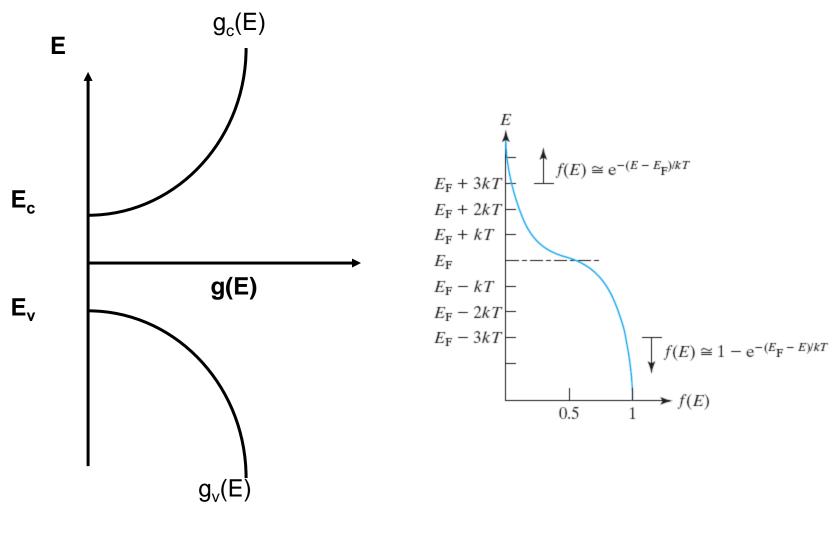


 $E_i = int rinsic Fermi level$ 

$$=\frac{1}{2}(E_{c}+E_{v})+\frac{3k_{B}T}{4}\ln\left(\frac{m_{p}^{*}}{m_{n}^{*}}\right)=E_{midgap}+\frac{3k_{B}T}{4}\ln\left(\frac{m_{p}^{*}}{m_{n}^{*}}\right)$$

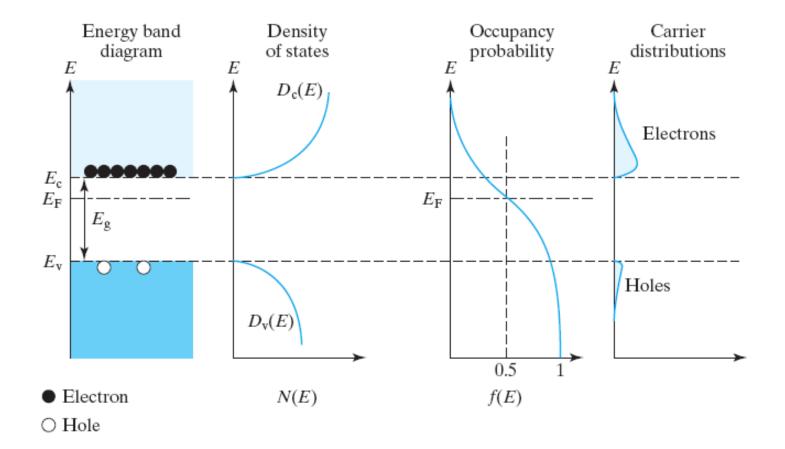
Neglecting the last term,

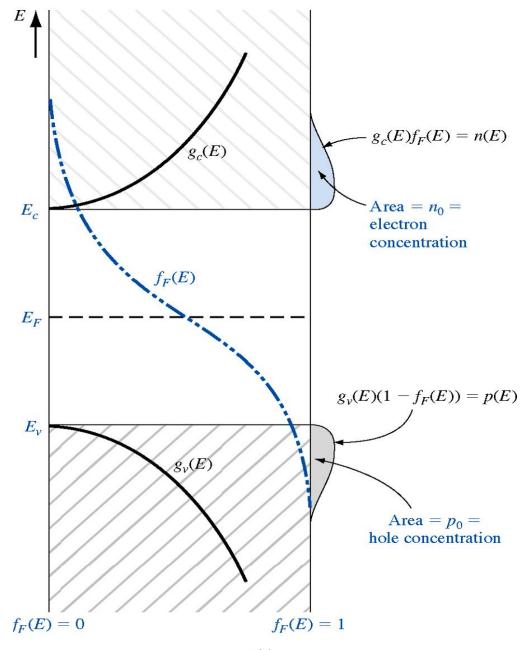
$$E_i = \frac{1}{2}(E_c + E_v)$$



DOS in CB & VB

**FD** function





#### Expressions for solving numerical on density of states, fermi distribution function and carrier concentration

$$g(E) = DOS = \frac{1}{V} \frac{dN}{dE}$$

$$g_c(E) = DOS \text{ in } CB = \frac{4\pi (2m_n^*)^{3/2}}{h^3} \sqrt{E - E_c}$$

$$g_v(E) = DOS \text{ in } VB = \frac{4\pi (2m_p^*)^{3/2}}{h^3} \sqrt{E_v - E}$$

$$f_F(E) = \frac{1}{1 + e^{\frac{E - E_F}{k_\beta T}}}$$

$$1 - f_F(E) = \frac{1}{1 + e^{\frac{E_F - E}{k_{\beta}T}}}$$

 $[kT]_{T} = [kT]_{300} \times T/300$ 

$$n_0 = N_c e^{-\frac{(E_c - E_f)}{k_B T}}$$

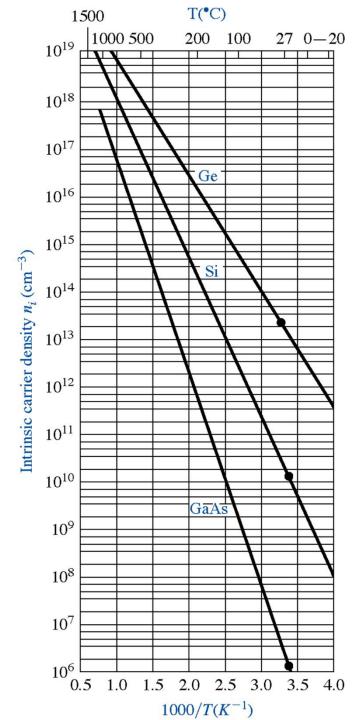
$$p_0 = N_v e^{-\frac{(E_f - E_v)}{k_B T}}$$

Table 4.1 | Effectivedensity of states function and eff

	$N_c ({\rm cm}^{-3})$	$N_v \ ({ m cm}^{-3})$
Silicon	$2.8 \ge 10^{19}$	$1.04 \times 10^{19}$
Gallium arsenide	$4.7 \times 10^{17}$	$7.0 \times 10^{18}$
Germanium	$1.04 \times 10^{19}$	$6.0 \times 10^{18}$

 $[N_{c}]_{T} = [N_{c}]_{300} X (T/300)^{3/2}$  $[N_{v}]_{T} = [N_{v}]_{300} X (T/300)^{3/2}$ 

$$n_{i} p_{i} = N_{c} N_{v} e^{-\frac{E_{c} - E_{v}}{k_{B}T}} = N_{c} N_{v} e^{-\frac{E_{g}}{k_{B}T}} = n_{i}^{2}$$
$$E_{fi} = \frac{1}{2} (E_{c} + E_{v}) + \frac{3k_{B}T}{4} \ln \left(\frac{m_{p}^{*}}{m_{n}^{*}}\right)$$



If the electron and hole effective masses are equal so that  $m_n^* = m_p^*$ , then the intrinsic Fermi level is exactly in the center of the bandgap. If  $m_p^* > m_n^*$  the intrinsic Fermi level is slightly above the center, and if  $m_p^* < m_n^*$  it is slightly below the center of the bandgap.

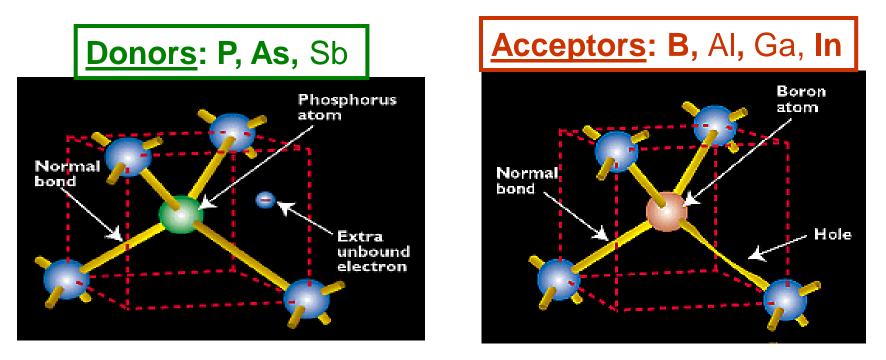
The intrinsic carrier concentration of Ge, Si, and GaAs as a function of temperature.

at T = 300 K

Silicon	$n_i = 1.5 \times 10^{10} \text{ cm}^{-3}$
Gallium arsenide	$n_{\rm r} = 1.8 \times 10^6  {\rm cm}^{-3}$
Germanium	$n_r = 2.4 \text{ x } 10^{13} \text{ cm}^{-3}$

#### **Donor & acceptor states**

In <u>extrinsic semiconductor</u>, controlled amounts of specific dopant or impurity atoms are added so that thermal-equilibrium electron and hole concentrations are different from the intrinsic semiconductor.



- As, a Group V element, introduces conduction electrons and creates Ntype silicon, and is called a donor.
- B, a Group III element, introduces holes and creates *P-type silicon*, and is called an *acceptor*.

### Ionisation Energy

 $E = T + V = -m^* e^4 / 8\pi^2 n^2 h^2$ 

- For Hydrogen E= -13.6 eV
- For Silicon E= 25.8meV is the energy required to lift an electron from donor level to conduction band
- Dopant ionization energy ~50meV (very low).

➢Silicon and germanium, can also be impurity atoms in gallium arsenide.

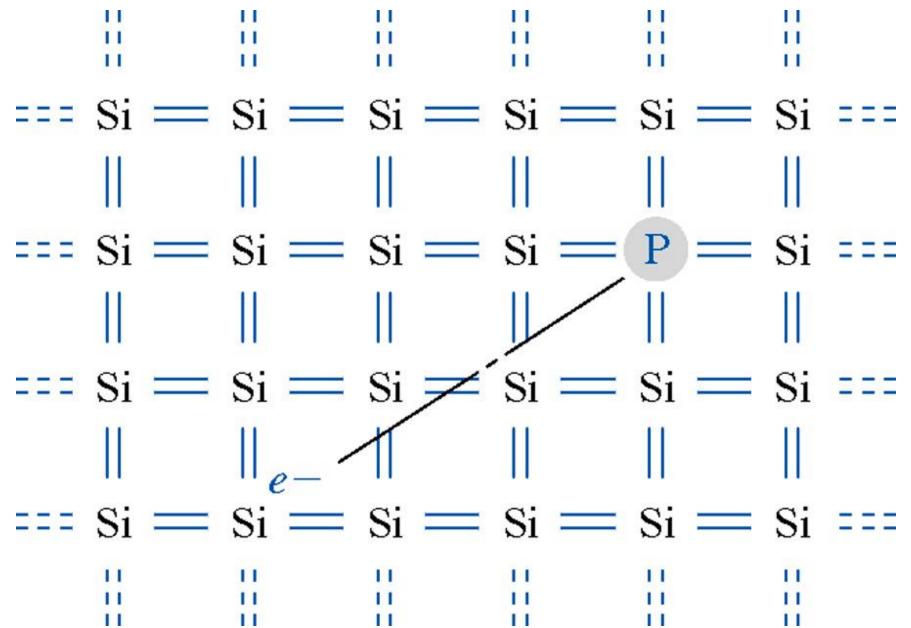
If a silicon atom replaces a gallium atom, silicon impurity will act as donor.

➢if the silicon atom replaces an arsenic atom, silicon impurity will act as an acceptor.

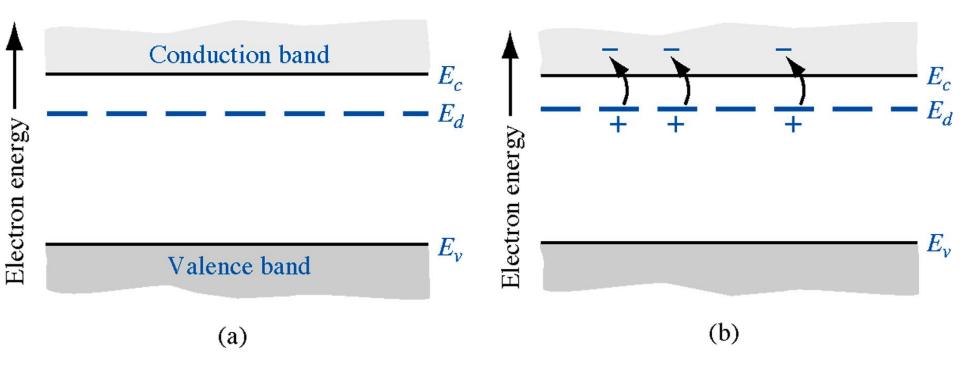
>The same is true for germanium as an impurity atom.

Such impurities are called *amphoteric*.

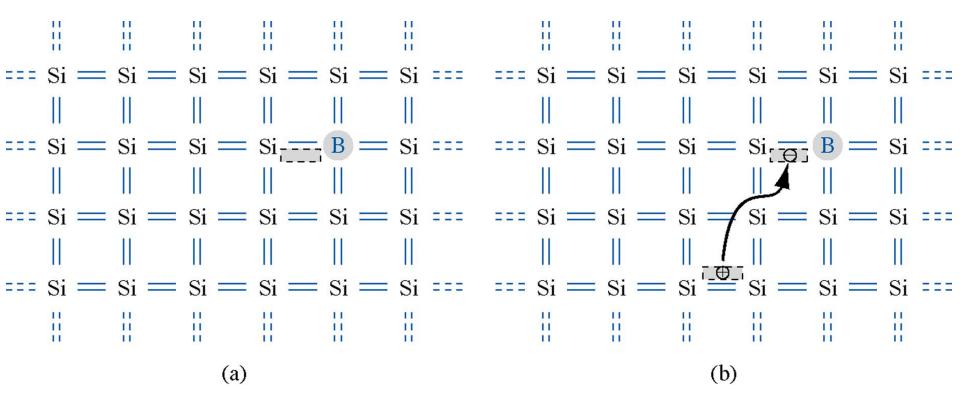
### **DONORS in Silicon crystal**



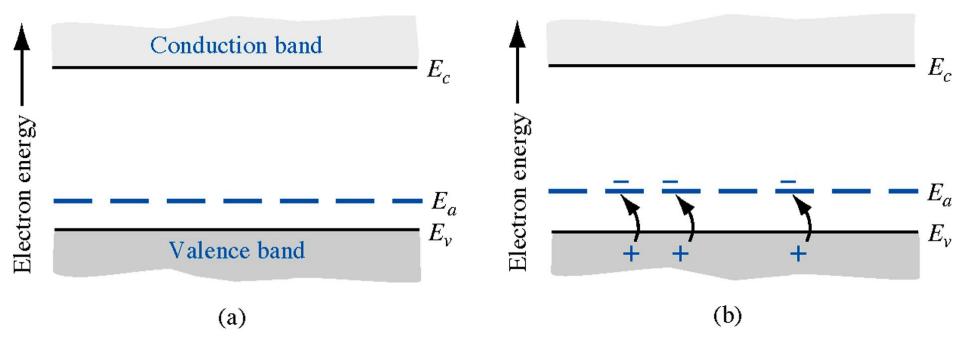
## **DONOR states in the band model**



### **ACCEPTORS in Silicon crystal**



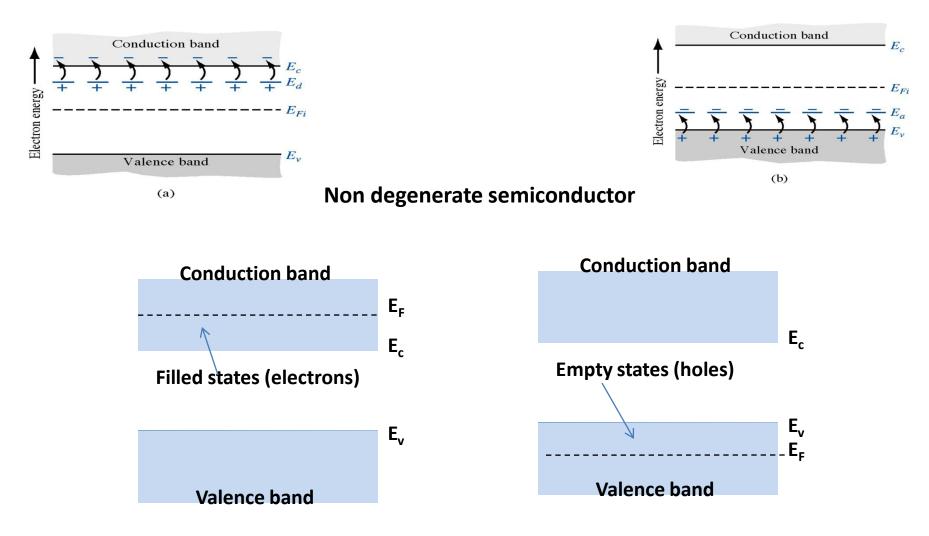
### ACCEPTOR energy states in the band model



# **Degenerate & nondegenerate semiconductors**

- When dopant conc. is small they are spread far apart from each other in the host, so there is no interaction between them.
- So, impurities introduces discrete, non interacting donor energy states in Ntype semiconductor and acceptor states in P-type semiconductor. **These are** called non degenerate semiconductors.
- But if the dopant conc. increases, the distance between them decreases, so they start interacting between themselves. This give rise to splitting in their energy level and formation of dopant energy bands
- For further increase in the dopant conc. i.e., for dopant conc. comparable with effective density of state  $N_c$  or  $N_v$ , dopant bands may overlap with the conduction band (for donor dopant) or valence band (for acceptor dopant) of the host semiconductor.
- Then the Fermi level may lie in the conduction / valence band. These are called degenerate semiconductors
- In degenerate n-type semiconductor, the states between  $E_F$  and  $E_c$  are mostly fill with electrons; so, the electron concentration in the conduction band is very high

Similarly, in the degenerate p-type semiconductor, the energy states between  $E_F$  and  $E_v$ , are mostly empty; so, the hole concentration in the valence band is very high



**Degenerate semiconductor** 

# **Carriers in Extrinsic Semiconductors**

 Dopants change the electron & hole distribution in semiconductor
 Fermi energy & Fermi level change in the band gap
 Electron & hole density in the CB & VB change
 If E<sub>F</sub> > E<sub>fi</sub>; then n<sub>0</sub> > p<sub>0</sub> ;- it is N-type, electrons are majority & holes are minority carrier
 If E<sub>F</sub> < E<sub>fi</sub>; then n<sub>0</sub> < p<sub>0</sub> ;- it is P-type, holes are majority

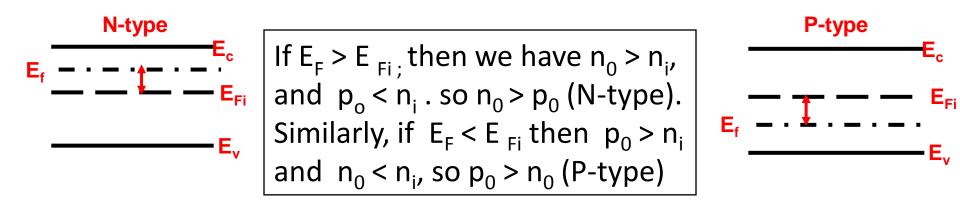
& electrons are minority carrier

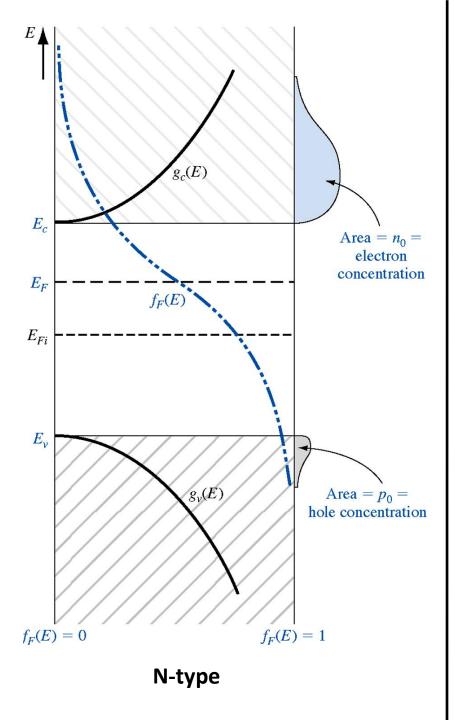
### Equilibrium Carrier concentration

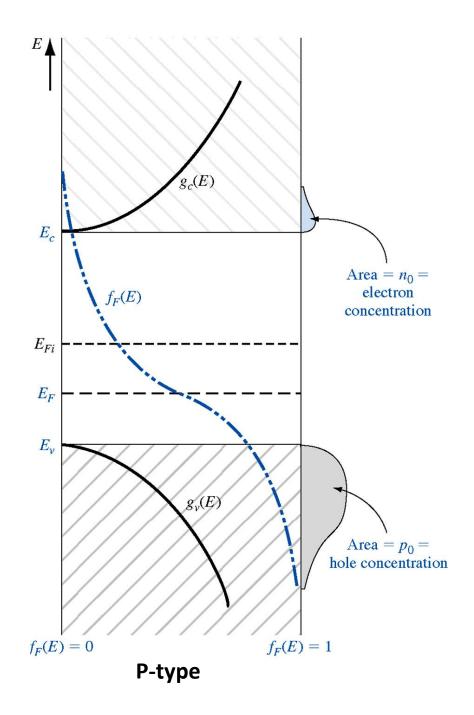
$$n_0 = N_c e^{-\frac{(E_c - E_f)}{k_B T}}$$
 &  $p_0 = N_v e^{-\frac{(E_f - E_v)}{k_B T}}$ 

$$n_{0} = N_{c}e^{-\frac{(E_{c}-E_{f})}{kT}} \text{ or, } n_{0} = N_{c}e^{\left[\frac{-(E_{c}-E_{Fi})+(E_{F}-E_{Fi})}{kT}\right]}$$
$$or, n_{0} = N_{c}e^{\left[\frac{-(E_{c}-E_{Fi})}{kT}\right]}e^{\left[\frac{(E_{F}-E_{Fi})}{kT}\right]}$$
$$so, n_{0} = n_{i}e^{\frac{(E_{F}-E_{Fi})}{kT}} similarly, p_{0} = n_{i}e^{-\frac{(E_{F}-E_{Fi})}{kT}}$$

$$n_0 p_0 = N_c N_v e^{-\frac{E_g}{k_B T}} = n_i^2$$







## **Complete Ionization, Partial ionization and Freeze-Out**

The probability function of electrons occupying the donor state is

$$n_d = \frac{N_d}{1 + \frac{1}{2} \exp\left(\frac{E_d - E_F}{kT}\right)}$$

• & 
$$n_d = N_d - N_d^+$$

• Similarly, 
$$p_a = \frac{N_a}{1 + \frac{1}{g} \exp\left(\frac{E_F - E_a}{kT}\right)} = N_a - N_a^-$$

• When

• 
$$(E_d - E_F) \gg kT$$
;  $n_d \approx \frac{N_d}{\frac{1}{2} \exp\left(\frac{E_d - E_F}{kT}\right)} = 2N_d \exp\left[\frac{-(E_d - E_F)}{kT}\right]$ 

$$n_0 = N_c \exp\left[\frac{-(E_c - E_F)}{kT}\right]$$
$$\frac{n_d}{n_d + n_0} = \frac{2N_d \exp\left[\frac{-(E_d - E_F)}{kT}\right]}{2N_d \exp\left[\frac{-(E_d - E_F)}{kT}\right] + N_c \exp\left[\frac{-(E_c - E_F)}{kT}\right]}$$

$$\frac{n_d}{n_d + n_0} \frac{1}{1 + \frac{N_c}{2N_d} \exp\left[\frac{-(E_c - E_d)}{kT}\right]}$$

 $(E_c - E_d)$  is the ionization energy of the donor electrons.

Ex:- If "P" is added to Si at 300K with conc.=  $10^{16}$  cm<sup>-3</sup> (E<sub>c</sub> - E<sub>d</sub>) = 0.045 eV

Ratio of electrons in the donor state to total electrons in CB plus donor electron =

$$\frac{n_d}{n_0 + n_d} = \frac{1}{1 + \frac{2.8 \times 10^{19}}{2(10^{16})} \exp\left(\frac{-0.045}{0.0259}\right)} = 0.0041 = 0.41\%$$

At RT, all the donor atoms have donated one electron to the conduction band or donor states are **completely ionised**, creating more electrons in the CB Similarly, all acceptor atoms have accepted an electron from the valence band, creating more holes in the VB i.e., there is **complete ionisation** in the acceptor states

At T= 0K, all electrons are in their lowest possible energy state; that is, for an n-type semiconductor, each donor state must contain an electron, therefore  $n_d = N_d$  or  $N_d^+ = 0$ 

So, 
$$exp\left(\frac{E_d - E_F}{kT}\right) = 0$$

As T=0, it happens when the numerator is = - $\infty$  or,  $E_F > E_d$ 

The Fermi energy level is above the donor energy level at absolute zero.

In p-type semiconductor at absolute zero temperature, the impurity atoms will not contain any electrons, so that the Fermi energy level must be below the acceptor energy state. The distribution of electrons among the various energy states, and Fermi energy, is a function of temperature. No electrons from the donor state are thermally elevated into the conduction band and no electrons from the valance band are elevated into the acceptor states. This effect is called **Freeze-out**. Between T = OK (freeze-out) & T = 300 K, complete ionization, there is partial ionization of donor or acceptor atoms.

# **Compensated Semiconductors**

- A compensated semiconductor contains both donor and acceptor impurity atoms in the same region. It is formed, by diffusing acceptor impurities into an n-type material, or by diffusing donor impurities into a p-type material.
- In n-type compensated semiconductor  $N_d > N_a$
- In p-type compensated semiconductor  $N_a > N_d$
- If N<sub>a</sub> = N<sub>d</sub> it is a completely compensated semiconductor having the characteristics of an intrinsic material.
- In thermal equilibrium, the semiconductor crystal is electrically neutral that is the net charge density is zero.

$$n_0 + N_a^- = p_0 + N_d^+$$
 As,  $n_d = N_d - N_d^+$ 

• Or, 
$$n_0 + (N_a - p_a) = p_0 + (N_d - n_d)$$
 &  $p_a = N_a - N_a^-$ 

 $n_{\rm d}$  and  $p_{\rm a}$  are the electron and hole conc. in the donor and acceptor states resp.

For **complete ionization**,  $n_d$  and  $p_a$  are both zero. So,

$$n_{0} + N_{a} = p_{0} + N_{d}$$

$$n_{0} + N_{a} = \frac{n_{i}^{2}}{n_{0}} + N_{d}$$

$$n_{0}^{2} - (N_{d} - N_{a})n_{0} - n_{i}^{2} = 0$$

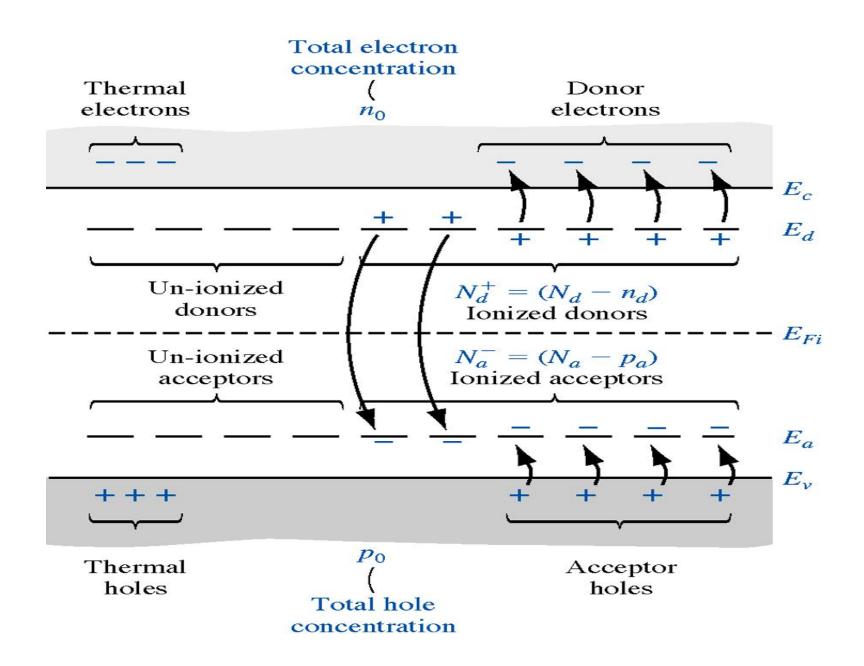
$$n_{0} = \frac{(N_{d} - N_{a})}{2} + \sqrt{\left(\frac{N_{d} - N_{a}}{2}\right)^{2} + n_{i}^{2}}$$

 $p_0 = \frac{n_i^2}{n_0}$ 

The positive sign in the quadratic formula must be used, since, in the limit of an intrinsic semiconductor when  $N_d = N_a = 0$ , the electron concentration must he a positive quantity, or  $n_0 = n_i$ .

similarily

$$p_0 = \frac{N_a - N_d}{2} + \sqrt{\left(\frac{N_a - N_d}{2}\right)^2 + n_i^2}$$



➤as we add donor impurity atoms, the conc. of electrons in the conduction hand increases above the intrinsic carrier concentration & minority carrier hole conc. decreases below the intrinsic carrier concentration

➢When donor impurity added, there is a redistribution of electrons among available energy states.

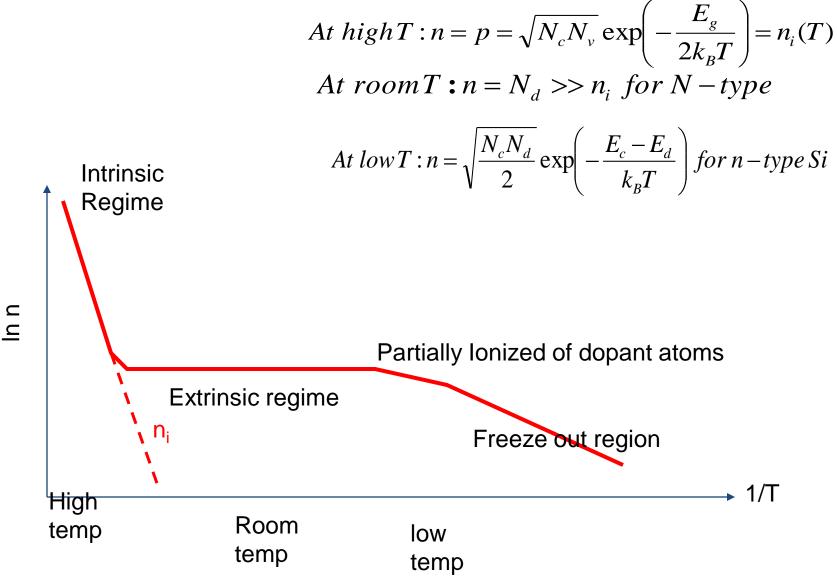
 $\geq$  A few of the donor electrons will fall into the empty states in the valence band and annihilate some of the intrinsic holes.

> The minority carrier hole concentration will therefore decrease

➢Also because of this redistribution, the net electron conc. in the conduction band is not equal to the donor concentration plus intrinsic electron concentration.

The intrinsic carrier concentration  $n_i$  is a very strong function of temp. As the temperature increases, additional electron-hole pairs are thermally generated so that the  $n_i$  term begin to dominate and the semiconductor will eventually lose its extrinsic characteristics.

## **Carrier Concentration and Temperature**



In N-type ; the majority carrier is calculated by

$$n_0 = \frac{(N_d - N_a)}{2} + \sqrt{\left(\frac{N_d - N_a}{2}\right)^2 + n_i^2}$$

& minority carrier by

$$p_0 = \frac{n_i^2}{n_0}$$

In P-type ; the majority carrier is calculated by

$$p_0 = \frac{N_a - N_d}{2} + \sqrt{\left(\frac{N_a - N_d}{2}\right)^2 + n_i^2}$$

& minority carrier by

$$n_0 = \frac{n_i^2}{p_0}$$

# Variation of Fermi level with dopant conc. and temp.

• We have,  

$$n_0 = N_c e^{-\frac{(E_c - E_f)}{k_B T}}$$

Or, 
$$E_c - E_F = kT \ln\left(\frac{N_c}{n_0}\right)$$

In N-type semiconductor,  $N_d \gg n_i$ , then  $n_0 \approx N_d$ 

So, 
$$E_c - E_F = kT \ln\left(\frac{N_c}{N_d}\right)$$

The distance between the bottom of the conduction band and the Fermi energy is a logarithmic function of the donor concentration. As the donor concentration increases, the Fermi level moves closer to the conduction band. Conversely, if the Femi level moves closer to the conduction band, then the electron concentration in the conduction band is increasing.

For, compensated semiconductor, then the  $N_d = N_d - N_{ar}$ 

as, 
$$n_0 = n_i e^{\frac{(E_F - E_{Fi})}{kT}}$$
  $E_F - E_{Fi} = kT \ln\left(\frac{n_0}{n_i}\right)$ 

Shows difference between the Fermi level and the intrinsic Fermi level as a function of the donor concentration. It is applicable for an n-type semiconductor, where  $n_0$ 

$$n_0 = \frac{(N_d - N_a)}{2} + \sqrt{\left(\frac{N_d - N_a}{2}\right)^2 + n_i^2}$$

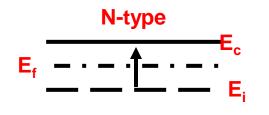
if  $N_d - N_a = 0$ , then  $n_0 = n_i$  and  $E_F = E_{Fi}$ 

$$again p_0 = N_v e^{-\frac{(E_f - E_v)}{k_B T}}$$

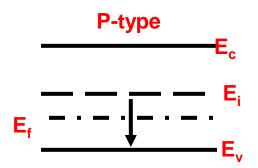
So, 
$$E_F - E_v = kT \ln\left(\frac{N_v}{p_0}\right)$$

and  $E_F - E_v = kT \ln\left(\frac{N_v}{N_a}\right)$ 

as the acceptor concentration increases, the Fermi level moves closer to the VB.



Fermi Energy, E<sub>f</sub>, moves towards conductance band on increasing doping.



Fermi Energy, E<sub>f</sub>, moves towards valance band on increasing doping.

Also, 
$$E_{Fi} - E_F = k_B T \ln \frac{p_0}{n_i}$$

Is applicable for an p-type semiconductor, where  $p_0$ 

$$p_0 = \frac{N_a - N_d}{2} + \sqrt{\left(\frac{N_a - N_d}{2}\right)^2 + n_i^2}$$

for an n-type semiconductor,  $n_0 > n_i$ , and  $E_F > E_{Fi}$ . The Fermi level for an n-type semiconductor is above  $E_F$ . For a p-type semiconductor,  $p_0 > n_i$ , so  $E_{Fi} > E_F$ . The Fermi level for a p-type semiconductor is below  $E_F$ .



## Variation of Fermi level with dopant conc. and temp.

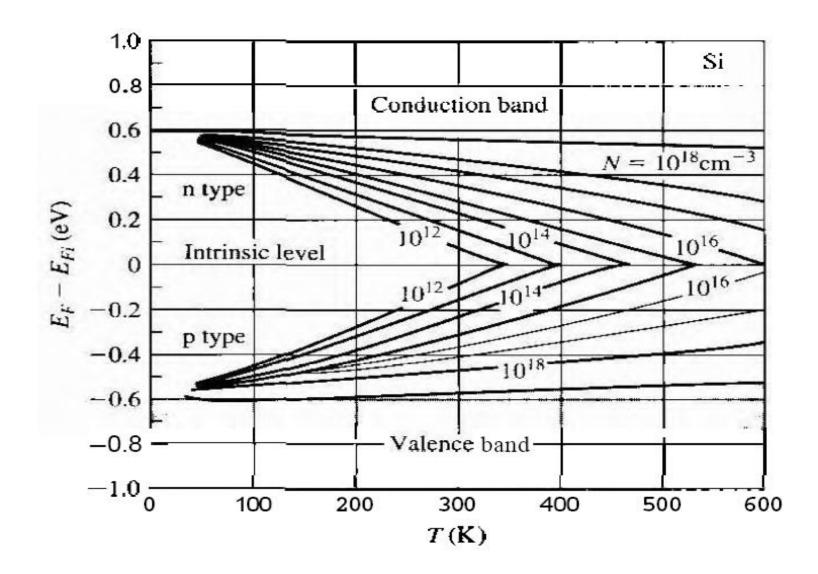
➢As the doping levels increase, the Fermi energy level moves closer to the conduction band for the n-type material and closer to the valence band for the p-type material

> As, n<sub>i</sub> depends on 'T' strongly, so also E<sub>F</sub>

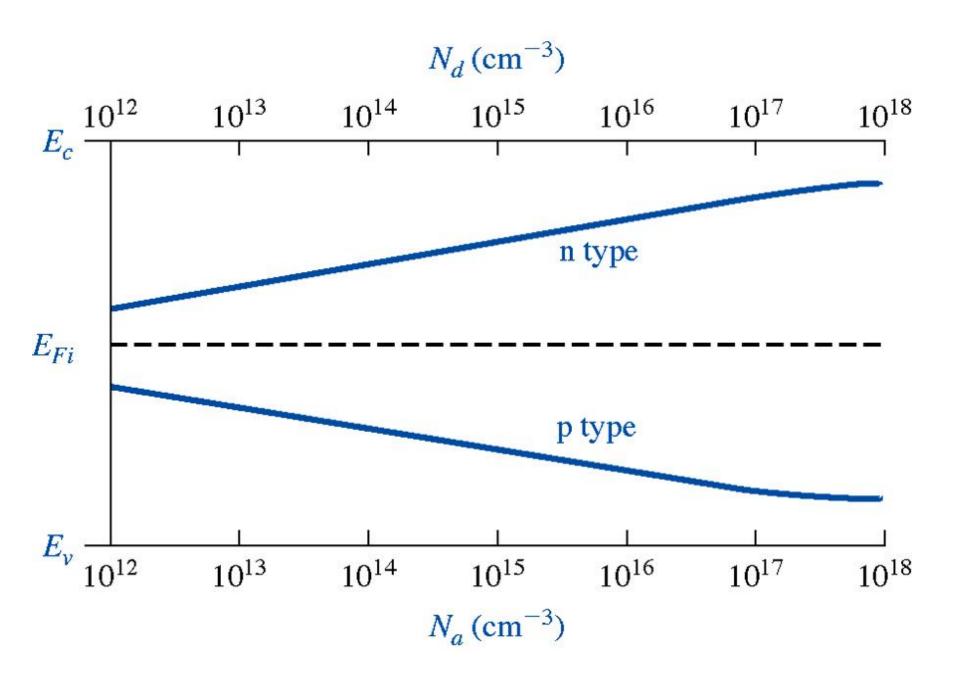
>As the temperature increases,  $n_i$  increases, and  $E_F$  moves closer to the intrinsic Fermi level.

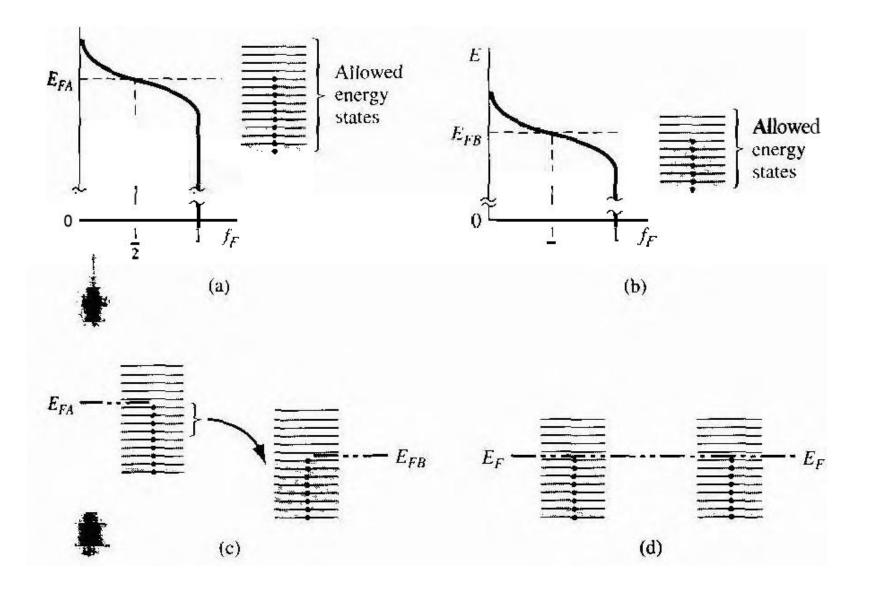
(i) At high temperature, the semiconductor material begins to lose its extrinsic characteristics and begins to behave more like an intrinsic semiconductor. So  $E_F = E_{Fi}$ (ii) At very low temperature, freeze-out occurs Then,  $E_F > E_d$  for the n-type and  $E_F < E_a$ , for the p-type material. (iii) At absolute zero degrees, all energy states below  $E_F$  are full and above  $E_F$  are empty.

➢In thermal equilibrium, the Fermi energy level is a constant throughout a system.

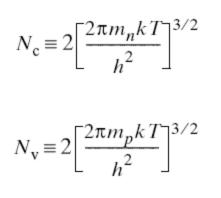


Position of Fermi level as **a function of** temperature for various doping concentrations.

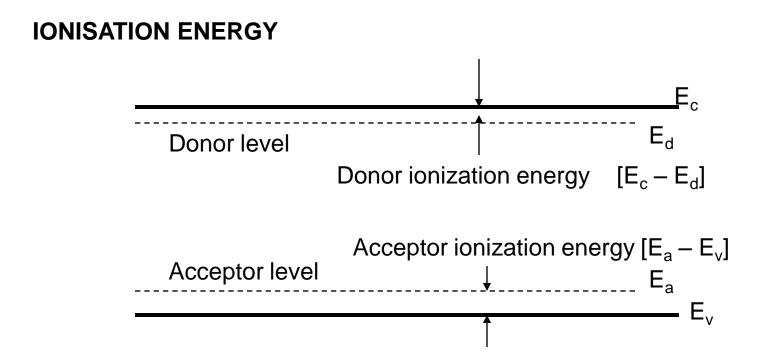




#### **EFFECTIVE DENSITY OF STATES**



It is as if all the energy states in the conduction band (valence band) were **effectively** squeezed into a single energy level, Ec (Ev), which can hold Nc(Nv) electrons (per cubic centimeter). As a result, the electron (hole) conc. is the product of Nc (Nv) and the probability that an energy state at Ec (Ev) is occupied (unoccupied).



#### Impurity ionization energies in silicon and germanium

Impurity	Ionization energy (eV)	
	Si	Ge
Donors		
Phosphorus	0.045	0.012
Arsenic	0.05	0.0127
Acceptors		
Boron	0.045	0.0104
Aluminum	0.06	0.0102

# Impurity lionization energies in gallium arsenide

Impurity	Ionization energy (eV)	
Donors		
Selenium	0.0059	
Tellurium	0.0058	
Silicon	0.0058	
Germanium	0.0061	
Acceptors		
Beryllium	0.028	
Zinc	0.0307	
Cadmium	0.0347	
Silicon	0.0345	
Germanium	0.0404	