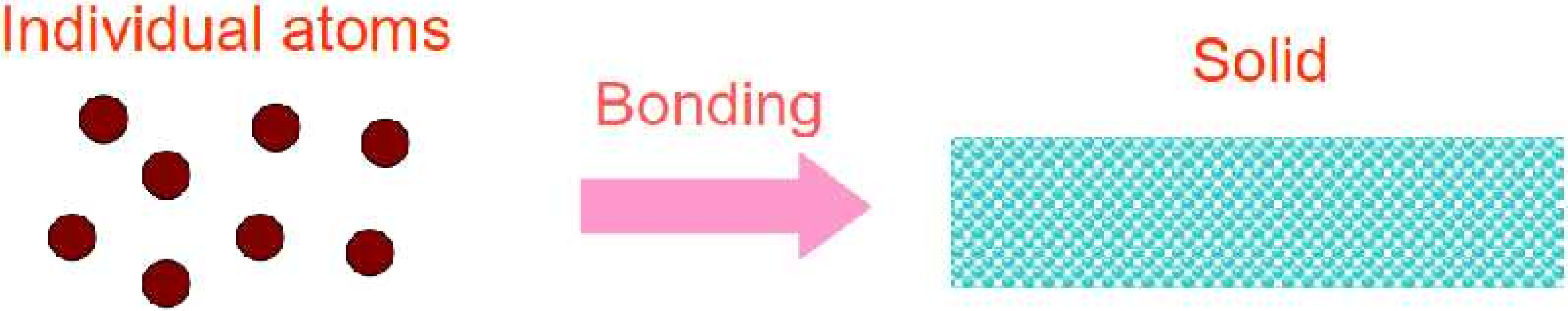
Ch. 2: **Energy Bands And Charge Carriers In Semiconductors**

Bonding Forces in Solids

Solids are made of large number of atoms brings together by bonding forces between these atoms



Individual atoms

Bonding

Solid

Bonding types in solids

- Ionic Bonding
- Metallic Bonding
- Covalent Bonding
- mixed ionic- covalent bonding

Ionic Bonding

A complete transfer of electron from one atom to another like NaCl

Na : $1s^2 2s^2 2p^6 3s^1$, Cl : $1s^2 2s^2 2p^6 3s^2 3p^5$

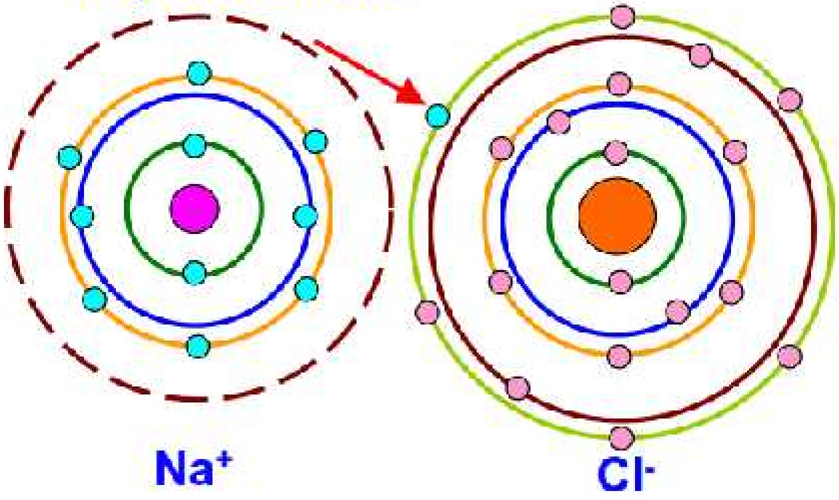
Na^+ : $1s^2 2s^2 2p^6$, similar to Ne (inert atom)

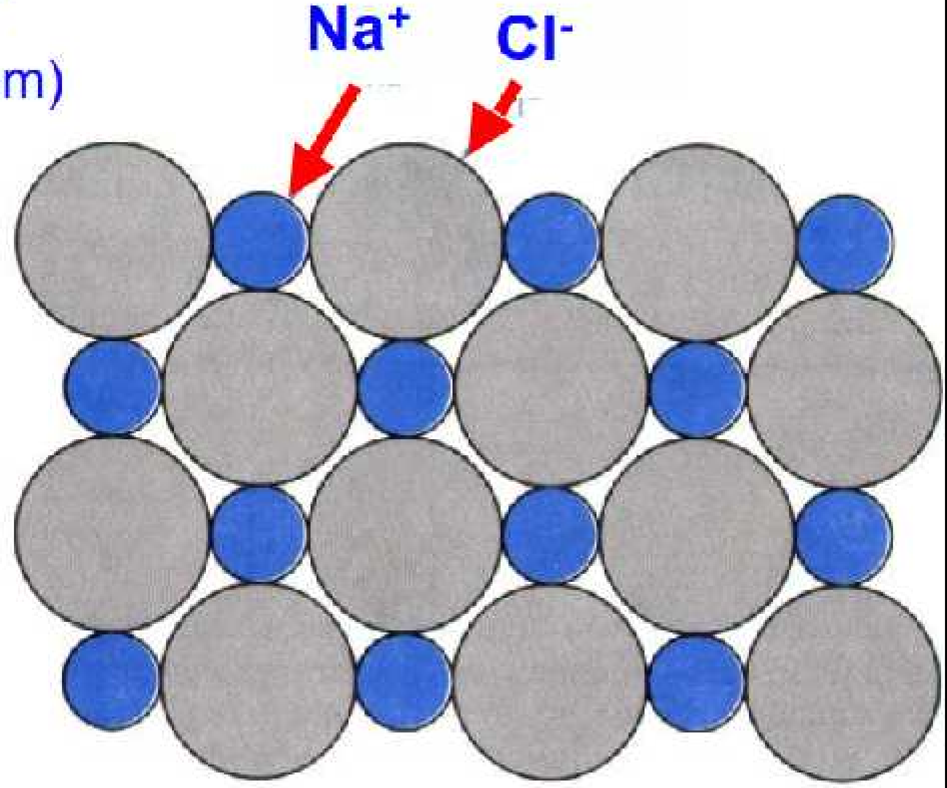
Cl^- : $1s^2 2s^2 2p^6 3s^2 3p^6$, similar to Ar

$Na^+ \leftrightarrow Cl^-$ Attractive force

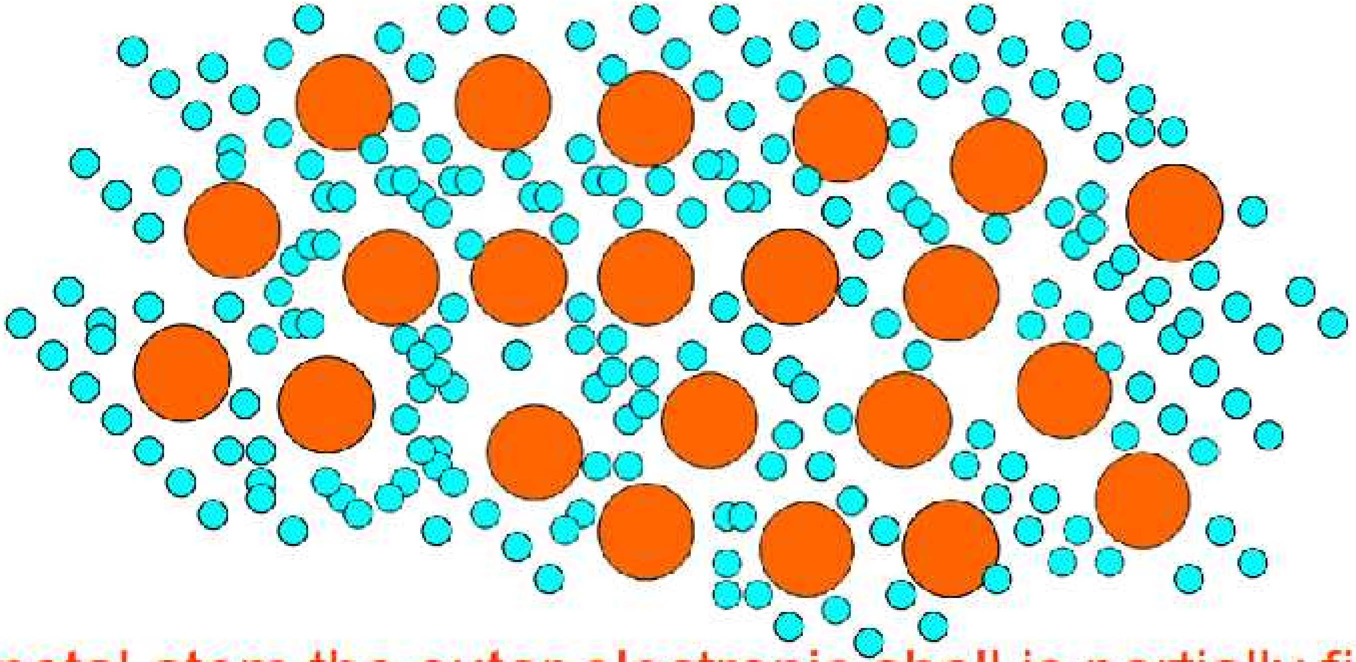
$Na^+ \leftrightarrow Na^+$ $Cl^- \leftrightarrow Cl^-$

Repulsive force





Metallic Bonding



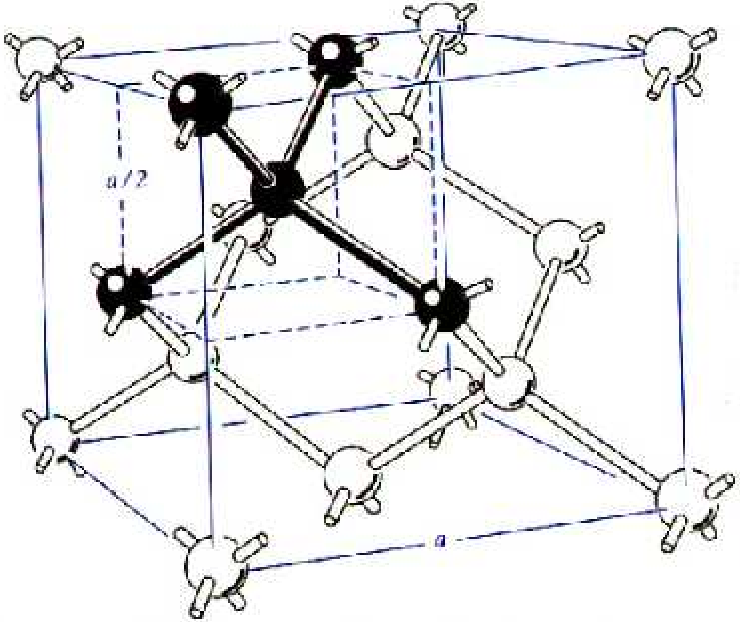
- In a metal atom the outer electronic shell is partially filled, usually by no more than three electrons

- Electrons in the outer electronic shell of atoms are loosely bound and are very easy to become free electrons to move around allm atoms in the solid.

Covalent Bonding

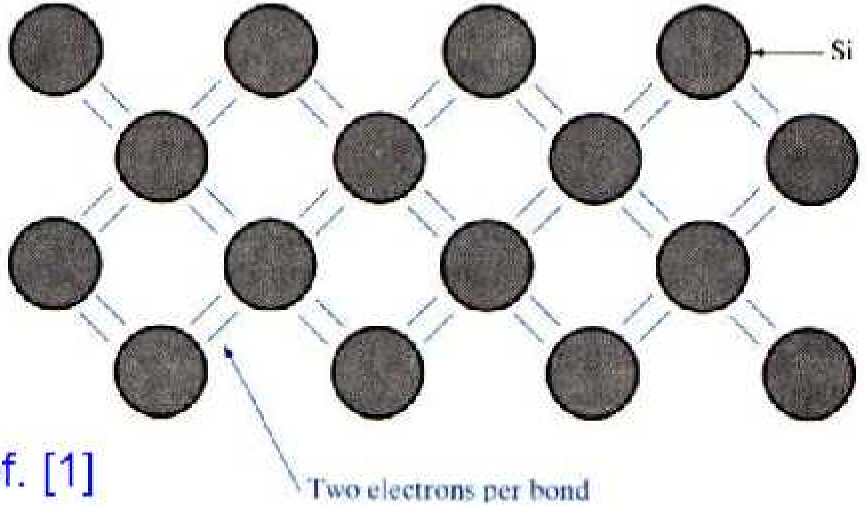
two atoms share one or more valence electron. each atom think it has a closed shell like:

Si $1s^2 2s^2 2p^6 3s^2 3p^2$, 4 electrons in the outer shells



Diamond lattice unit cell, showing the four nearest neighbor structure.

Ref. [1]

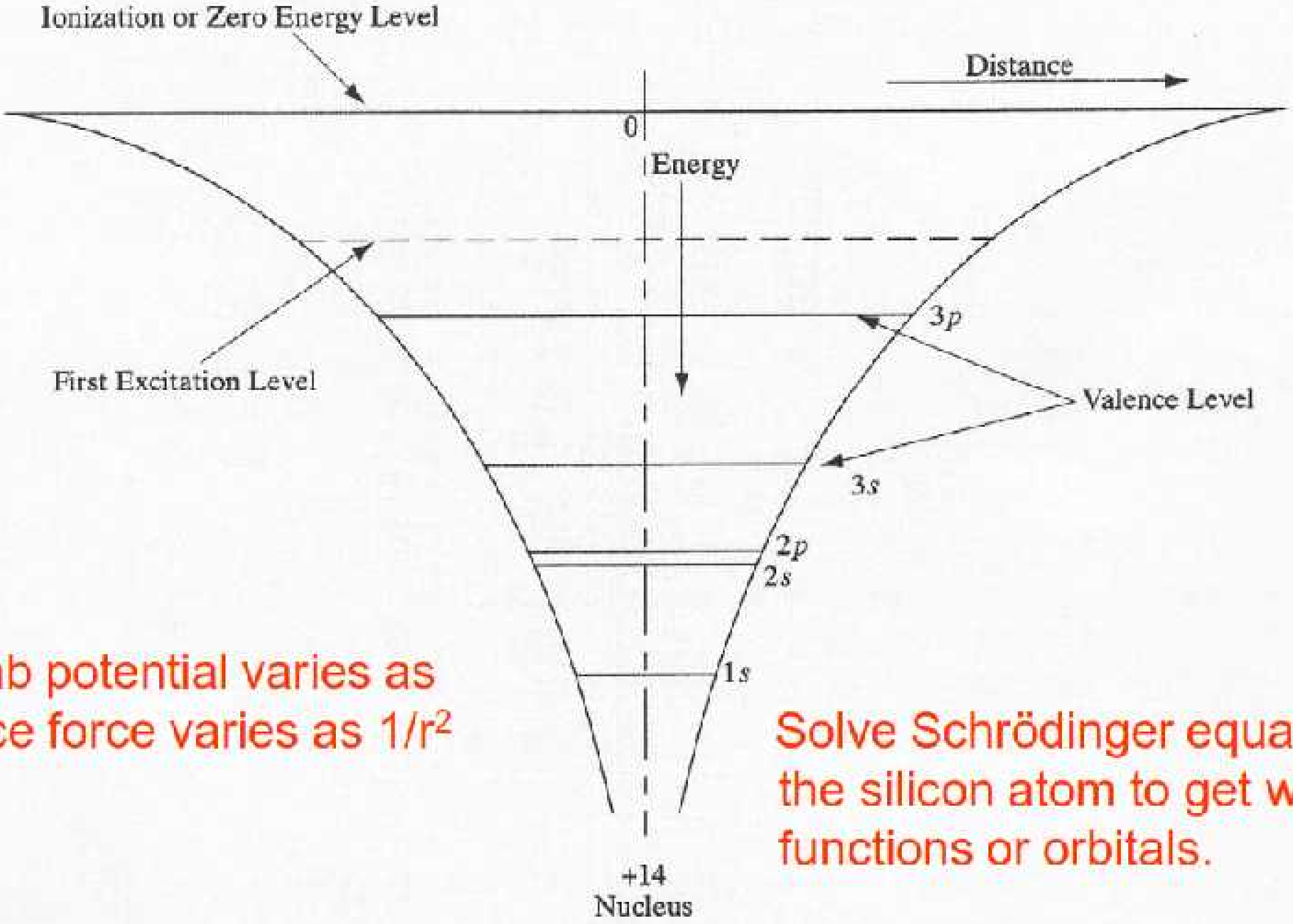


Covalent bonding in the Si crystal, viewed along a <100> direction.

Compound semiconductors such as GaAs have mixed bonding, in which both ionic and covalent bonding forces participate.

Energy Levels of Silicon

discrete energy levels for an atom is caused by the potential well around the nucleus as shown



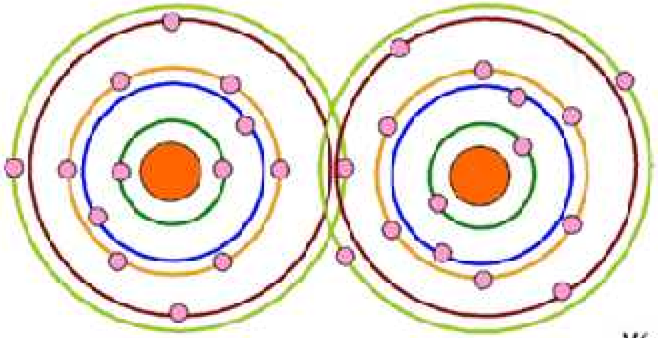
Coulomb potential varies as 1/r, since force varies as $1/r^2$

Solve Schrödinger equation for the silicon atom to get wave-functions or orbitals.

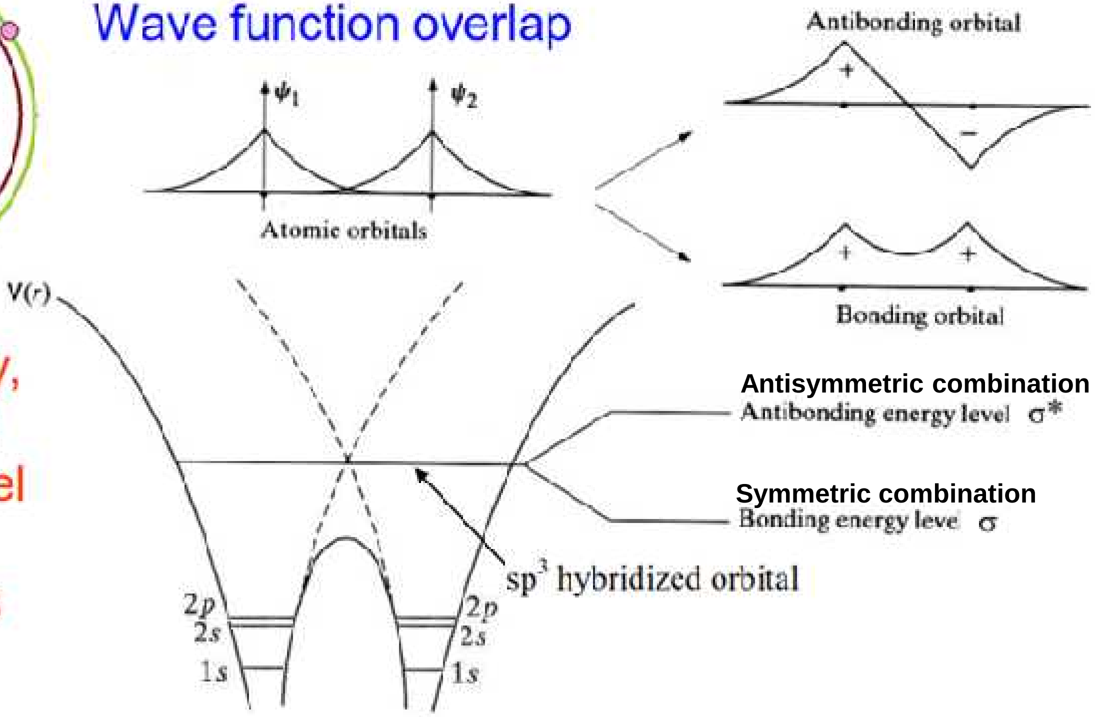
Discrete energy levels arise from balance of attraction force between electrons and nucleus and repulsion force between electrons → each electron will have it's own energy level

Linear Combinations of Atomic Orbitals (LCAO) (1)

How the wave functions and energy levels are modified when atoms are close to each other?



Wave function overlap



Antisymmetric combination

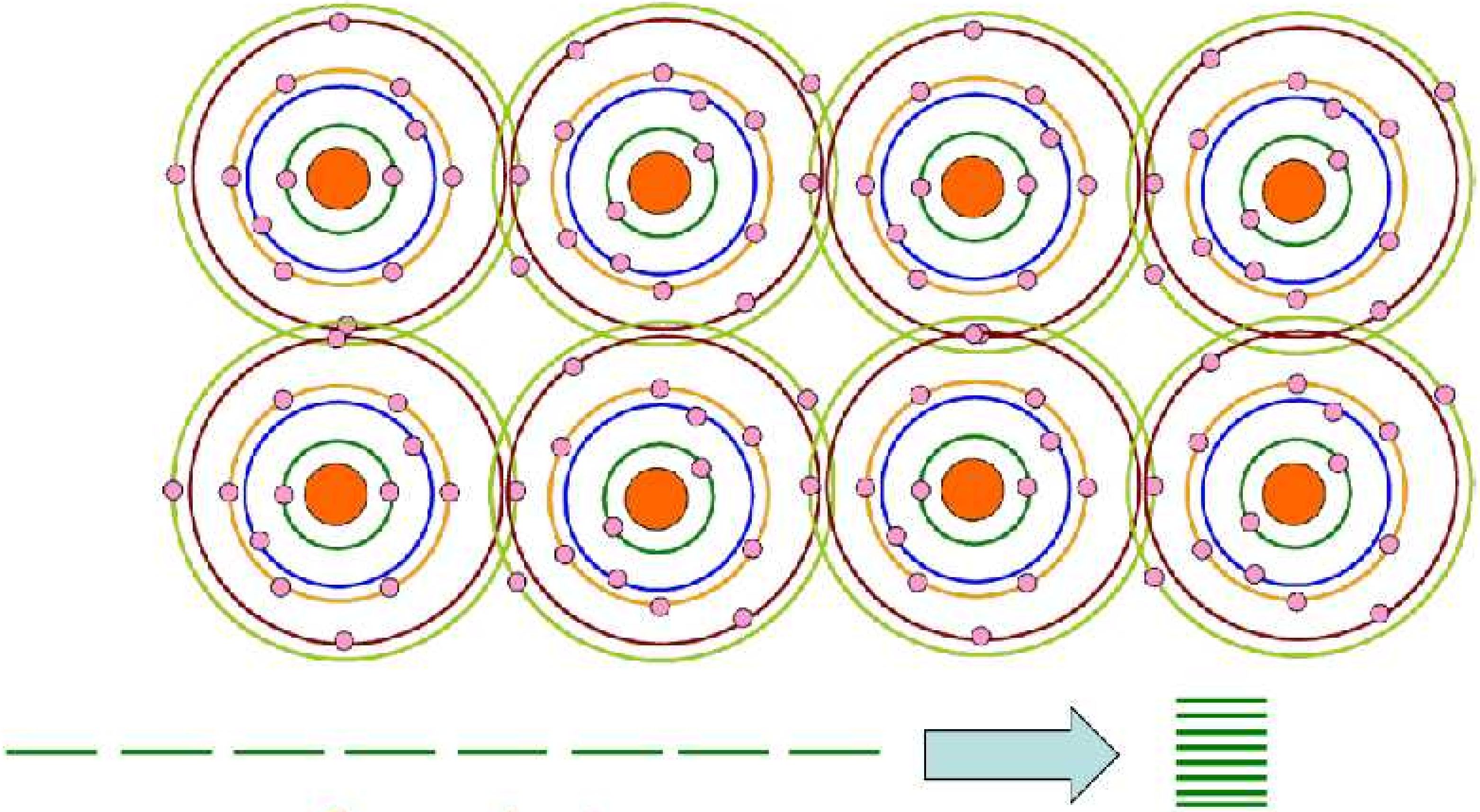
Symmetric combination

As the atoms come close by, the electron wave functions overlap, and the energy level splits to accommodate the electrons and satisfy Pauli's exclusion principle.

Pauli's exclusion principle: Identical energy states split to have an energy state for each electron

When two atoms brought together → two distinct modes: 1- higher energy anti-bonding orbital σ*
2- lower energy bonding orbital σ

LCAO (2): Splitting of single energy orbitals



8 separate atoms

Bond together

A single energy level will split into 8

LCAO (3)

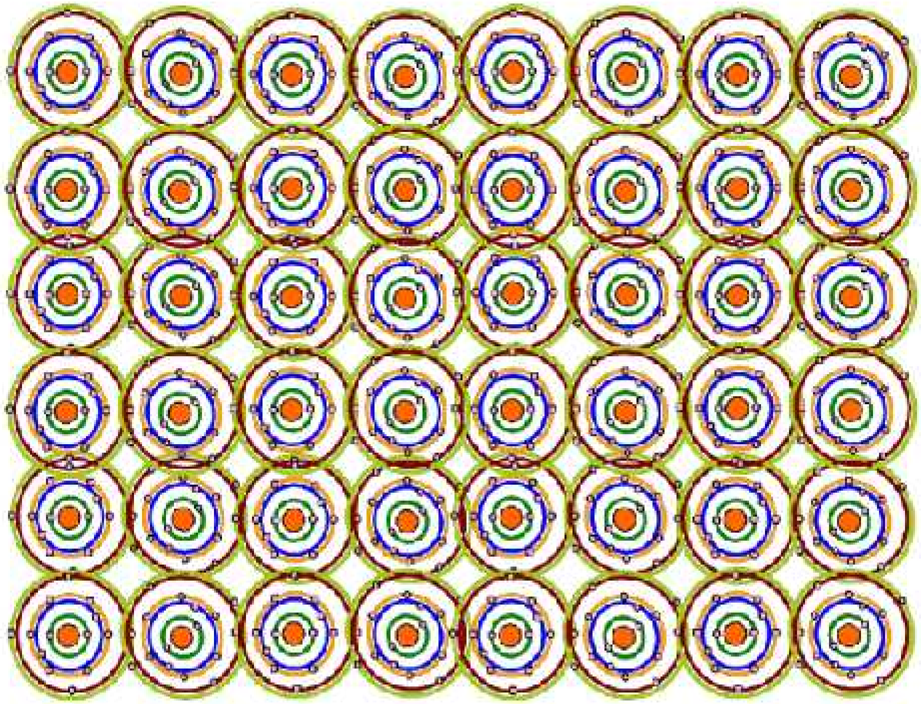
For N separate interacting atoms, each energy level in an isolated atom will split into N levels.

If N is a very large number, then the N levels will form an energy band.

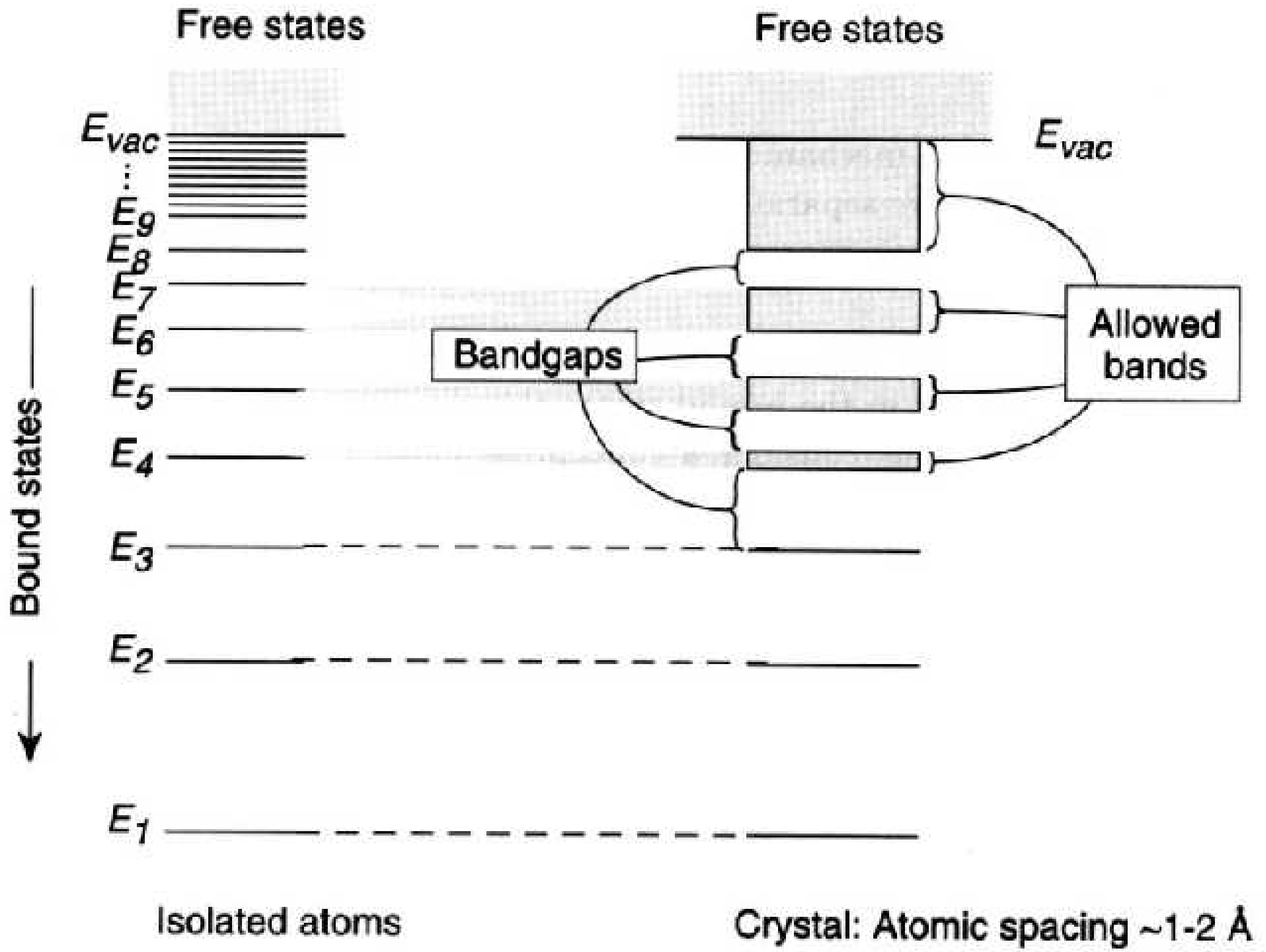
Energy band

N ×

Bond together



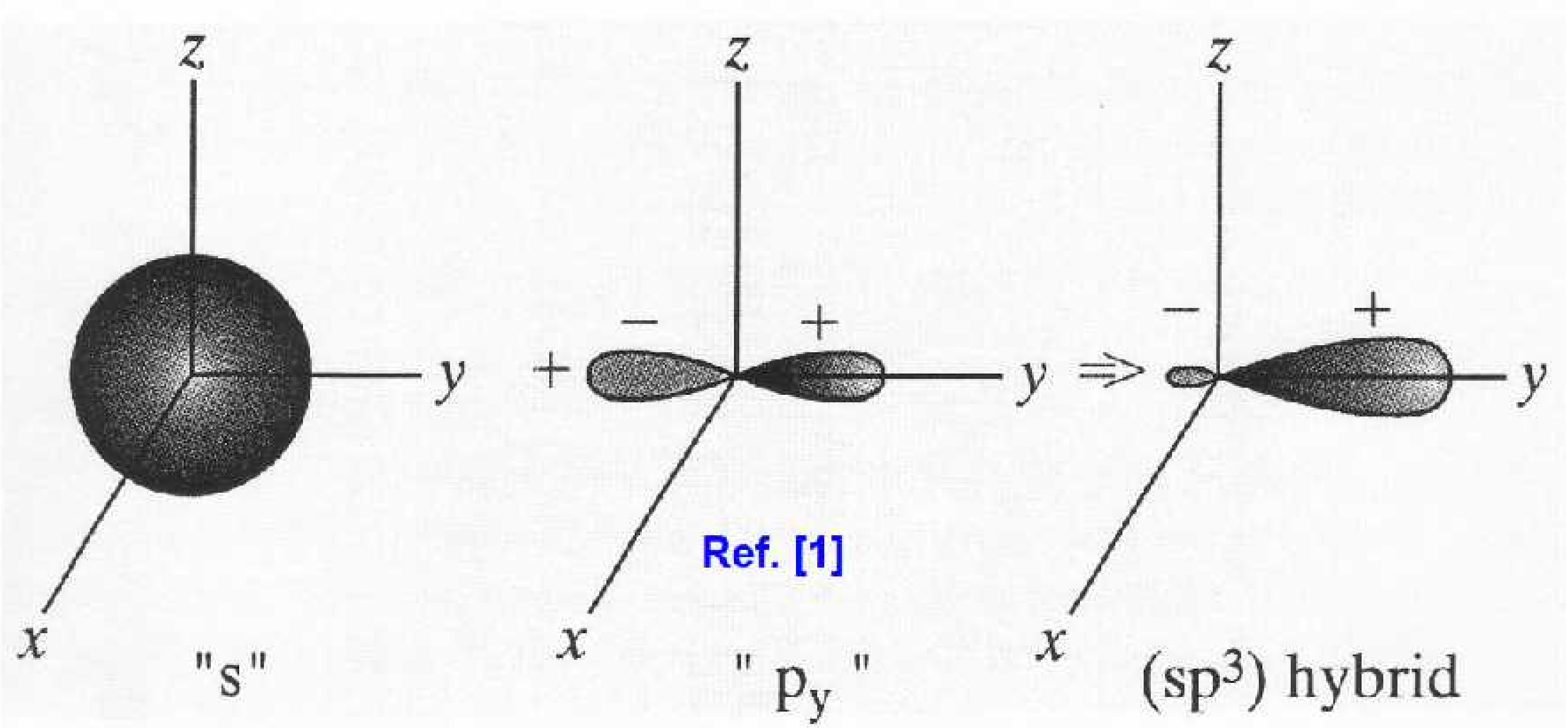
LCAO (4)



Note: Each energy state for an isolated atom gives rise to bands

Bands formation in Si

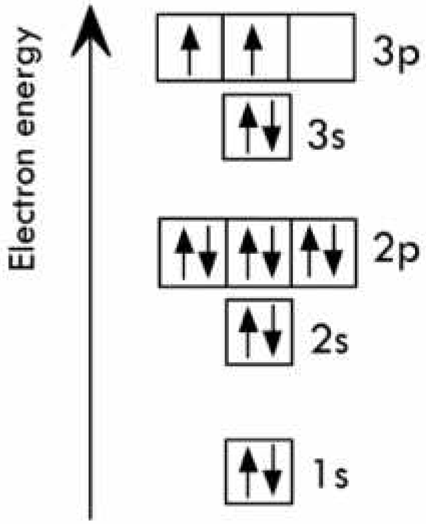
sp^3 Hybridization in Si



Ref. [1]

When individual atoms are very close together, the s and p-orbitals in adjacent atoms overlap so much that they can form hybridized orbitals. For example: 1s and 3p orbitals can mix to give sp^3 hybridized orbitals

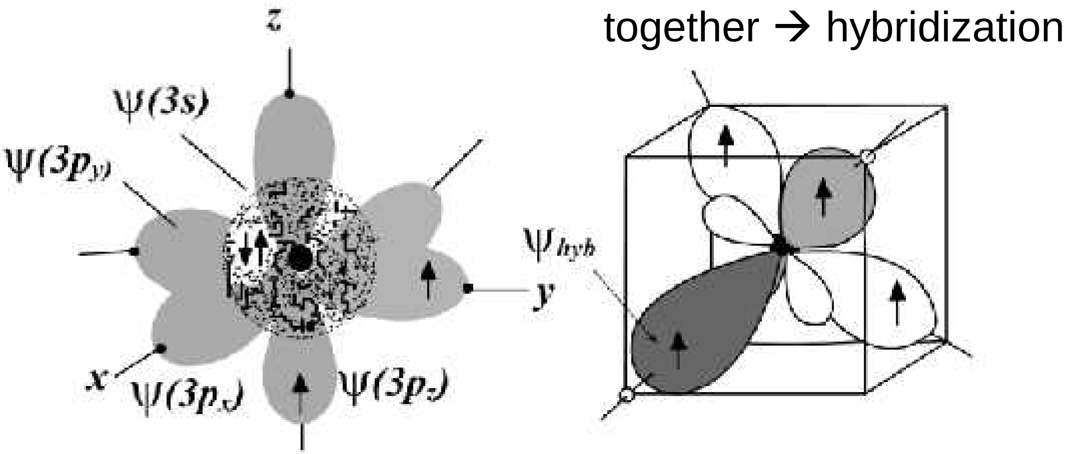
Bands formation in Si



Electronic configuration of Si atom.

The 3*s* and 3*p* together forms the outer shell

When atoms become close together → hybridization



(a) Isolated Si **(b) Si just before bonding**

(a) Isolated Si atoms showing the outer shell orbitals. (b) In a solid, these orbitals hybridize to form 4 sp^3 orbitals, just before bonding.

Bands formation in Si

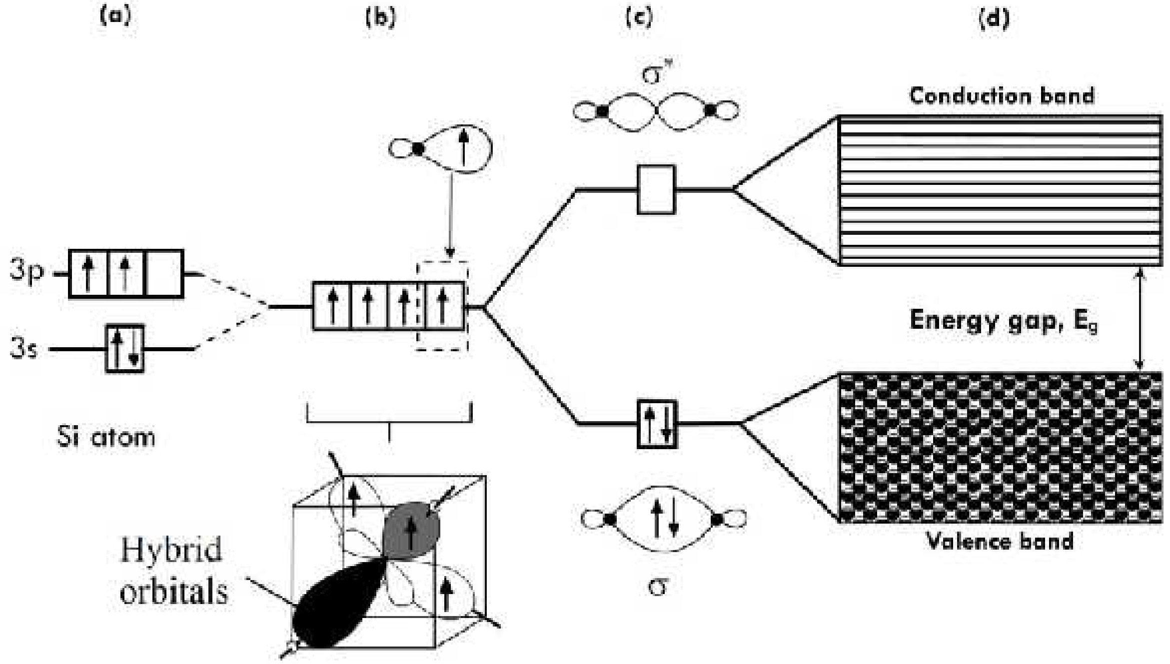
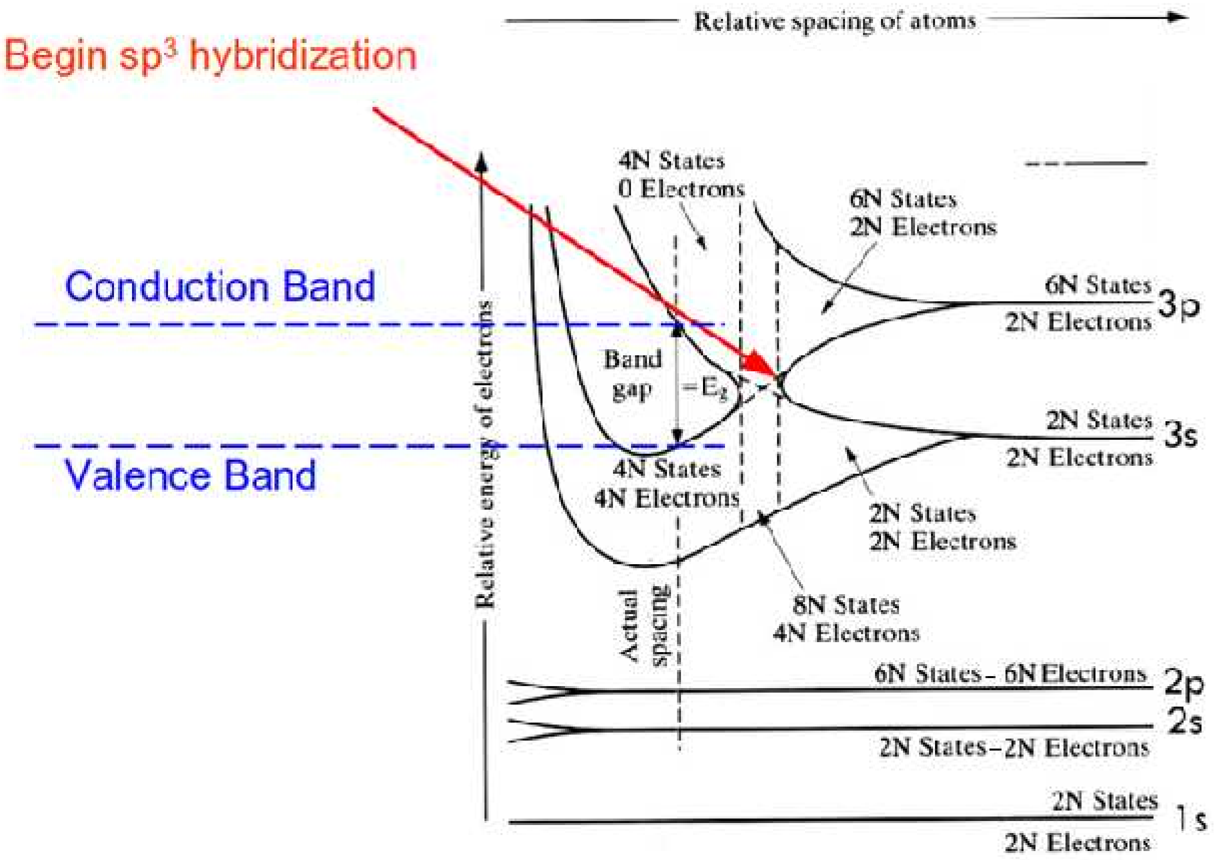


Figure 4: Formation of energy bands in Si when Si atoms approaches each other. (a) Si atom with 4 electrons in outer shell form (b) 4 sp^3 hybrid orbitals. (c) The hybrid orbitals form σ and σ^* orbitals. (d) These orbitals overlap in a solid to form the valence and conduction band.

1st sp^3 orbital in a given Si atom interacts with sp^3 orbital from other Si atom. 2nd sp^3 orbital the given Si atom will interact with other sp^3 orbital from other second Si atom, and so on with other sp^3 orbitals in the given Si atom→ the 4 sp^3 orbitals in a given Si atoms need 4 other Si atom to form a bonded Si solid → in a solid of N Si atoms, each atom is bonded to four other Si atoms. This interaction will create a band (V. B) from σ orbitals full of electrons, and other band (C.B) from σ^* orbitals empty from electrons. These bands are separated by an energy gap (E_g)

Bands formation in Si

Formation of Energy Bands in Si

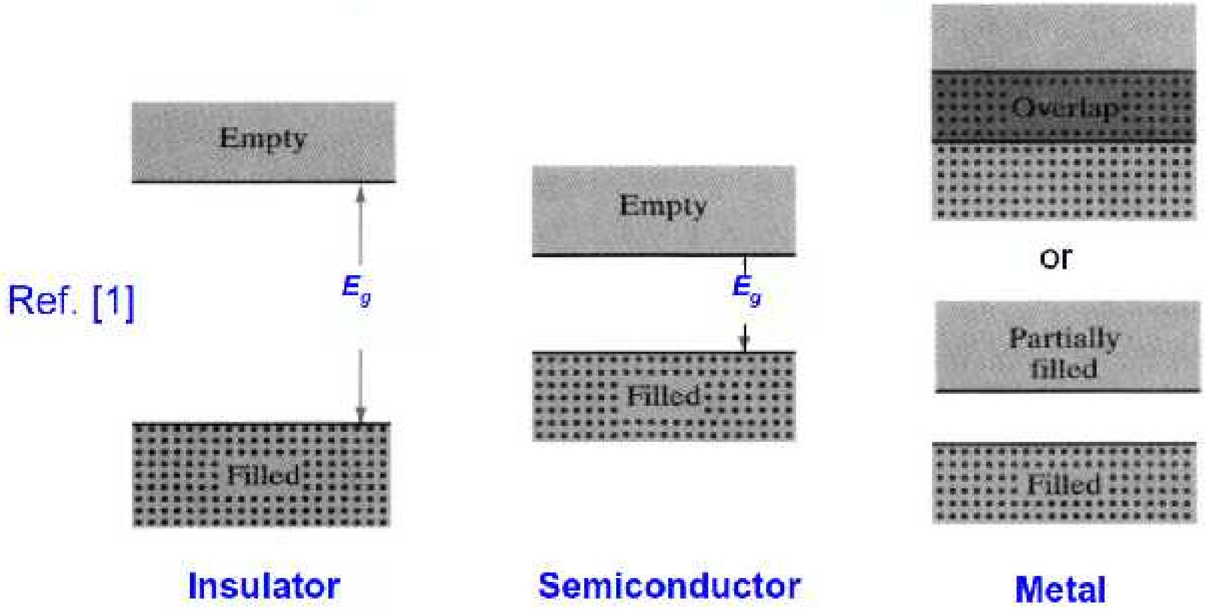


1) For N Si atoms, we have 14 N electrons distributed over 18 N states as shown
2) When atoms becomes close together → hybridization of outer shell to sp3 orbitals
3) splitting of orbitals into valence band (4 N lower states full of electrons) and conduction band (4 N upper states empty)

As distance reduces the bands first mix among themselves, then hybridize (mix), and then for even lower distance splits into conduction and valence bands

Metals, Semiconductors, and Insulators

(Electron distribution at T = 0 K)



- At T = 0 K, Semiconductor has same structure as insulator → filled valence band and empty conduction band→ no current will occur when applying E field. This is because no empty states in the valence band → no net motion of electrons.

Available Electron States → Motion of Electrons → Conduction

- The difference between insulators and Semiconductors is the E_g (for semiconducting Si Eg = 1.1 eV and for insulating diamond Eg = 5 eV).
- In semiconductors at room temperature, electrons can be excited thermally across the energy gap into the conduction band.→ Conductivity occurs due to available states in the C.B.
- Insulators has a negligible no. of free electrons at room temperature → almost no conductivity
- In metals, C.B and V.B. overlabs → electrons can move freely even at 0 K

Direct and Indirect Semiconductors: Concept of k-space 1

Solution of Schrödinger Equation for an Electron in a Periodic Lattice is given as:

Electron wave function $\Psi_k(x) = U(k_x, x)e^{jk_x x}$

k is the propagation constant or called the wave vector

where $\hbar k$ the momentum of the electron, and $U(k_x, x)$ is a periodic potential function based on the lattice periodicity.

Electron wave-function: $\psi(x) \sim e^{jkx}$

CRUDE UNDERSTANDING: (assuming electrons are free, which actually they are not, but they behave like free due to crystal forces):

	Classical variable	**Quantum operator**
	x	***x***
	f(x)	***f(x)***
	p(x)	$\frac{\hbar}{j}\frac{\partial}{\partial x}$
Total energy	***E***	$-\frac{\hbar}{j}\frac{\partial}{\partial t}$
Kinetic energy	$\frac{p^2(x)}{2m}$	$\frac{1}{2m}\left(\frac{\hbar}{j}\frac{\partial}{\partial x}\right)^2 = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$

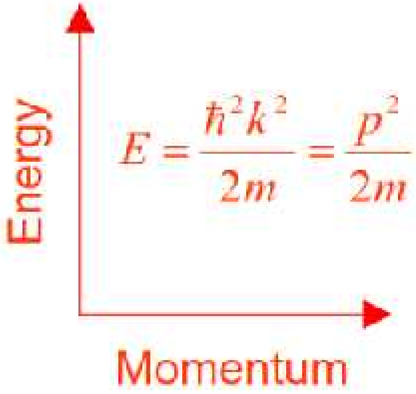
So, the Kinetic energy operator applied on the wave-function gives: $\hbar^2 k^2 / 2m$

And the momentum operator gives: $\hbar k$

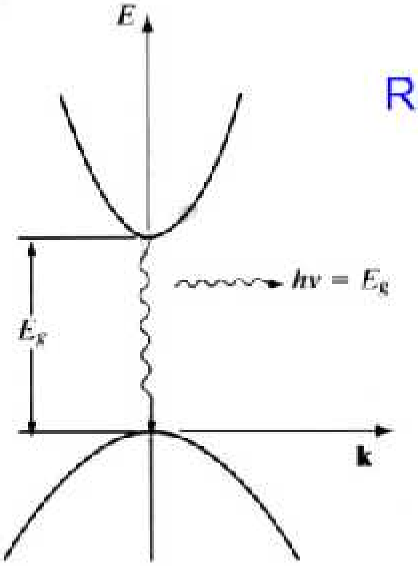
Two different plots raised from plotting E and k → complex 3-D surface

Direct and Indirect Semiconductors: Concept of k-space 2

In Energy - Momentum (E-k) Space: 2-D draw - parabola

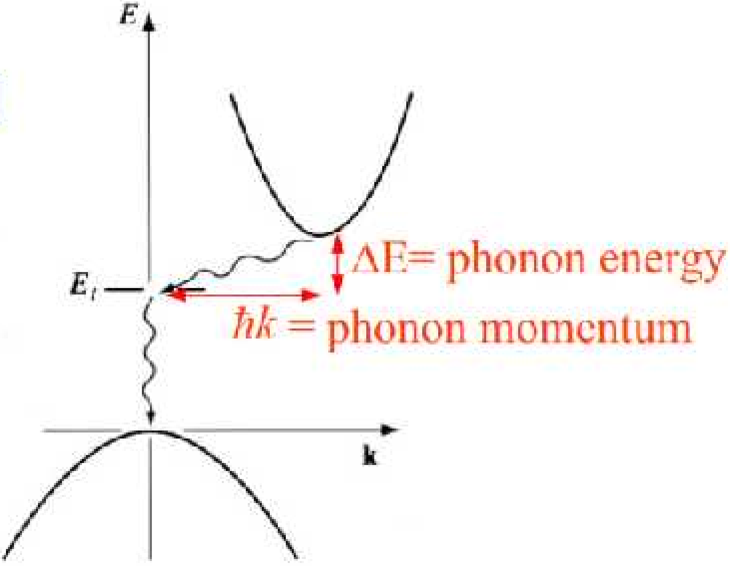


$$E = \frac{\hbar^2 k^2}{2m} = \frac{p^2}{2m}$$



Direct Bandgap

Ref. [1]



Indirect Bandgap

Note the parabolic relation between the energy and the wavefunction

Direct and Indirect Semiconductors

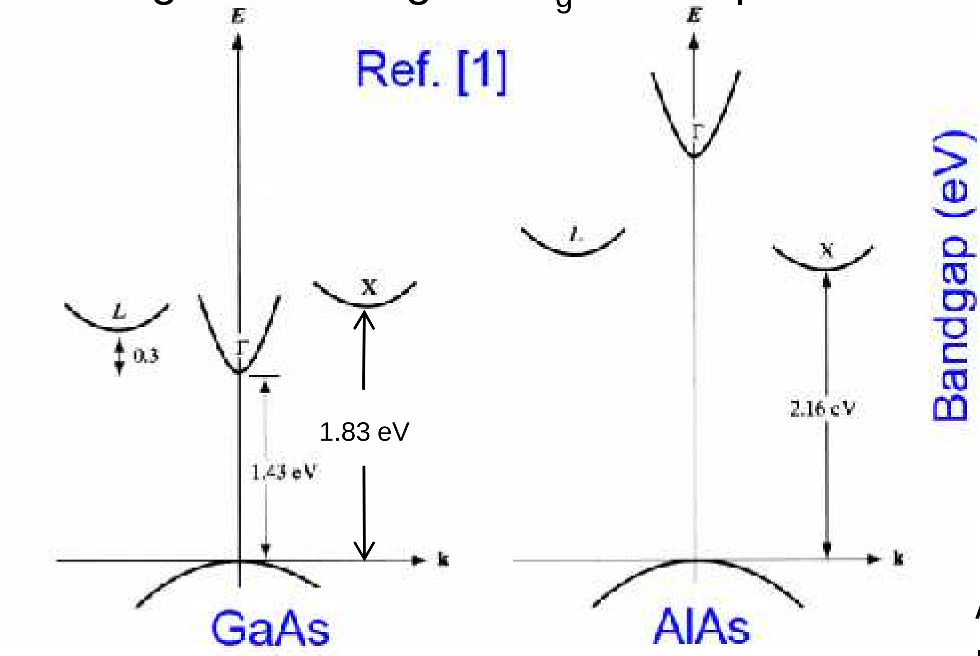
Direct Semiconductors: Electrons can make a smallest-energy (bandgap) transition from the conduction band to the valence band without a change in *k* value, i.e. without change in momentum. Such direct transitions give rise to particles called Photons.

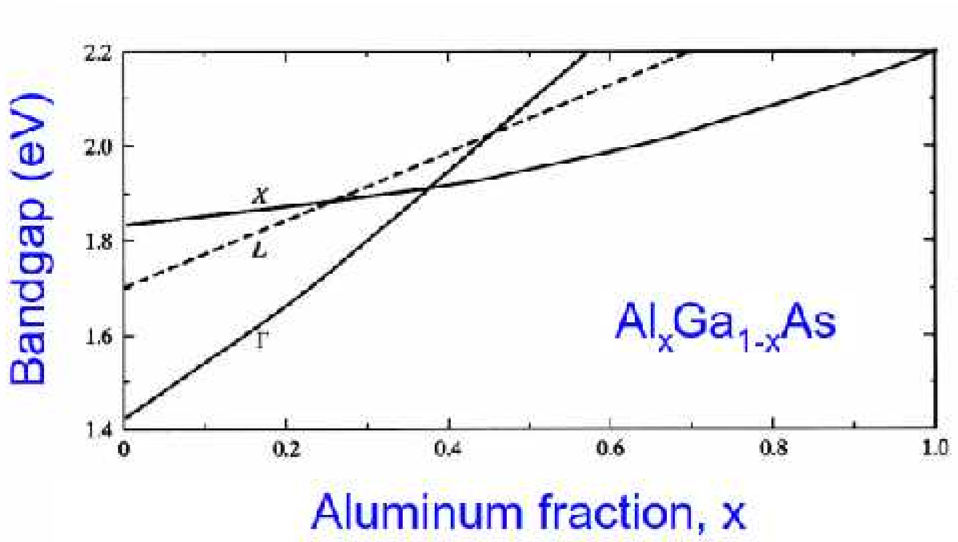
Indirect Semiconductors: Electrons cannot make the smallest-energy transition from the conduction band to the valence band without a change in *k* value (i.e. momentum which is $\mathrm{h}k$). Electrons must undergo a change of *k* value first. The change of *k* value will result from either losing or gaining energy from the lattice vibrations or Phonons. Since two particles are needed for such a transition, the probability is very low. Therefore, the probability of photon emission, i.e. light efficiency, will be very low. Electron-hole pairs in indirect bandgap material recombine through other processes to create more lattice vibrations or heat.

Both energy and momentum needs to be conserved during transitions. If transition is vertical there is no momentum change, but if it is not vertical, then there is a momentum change which needs to be accounted for.

Variation of Energy Bands with Alloy Composition

III-V ternary and quaternary compounds varies in composition → Band structure changes → change in E_g : Example GaAs doped with Al



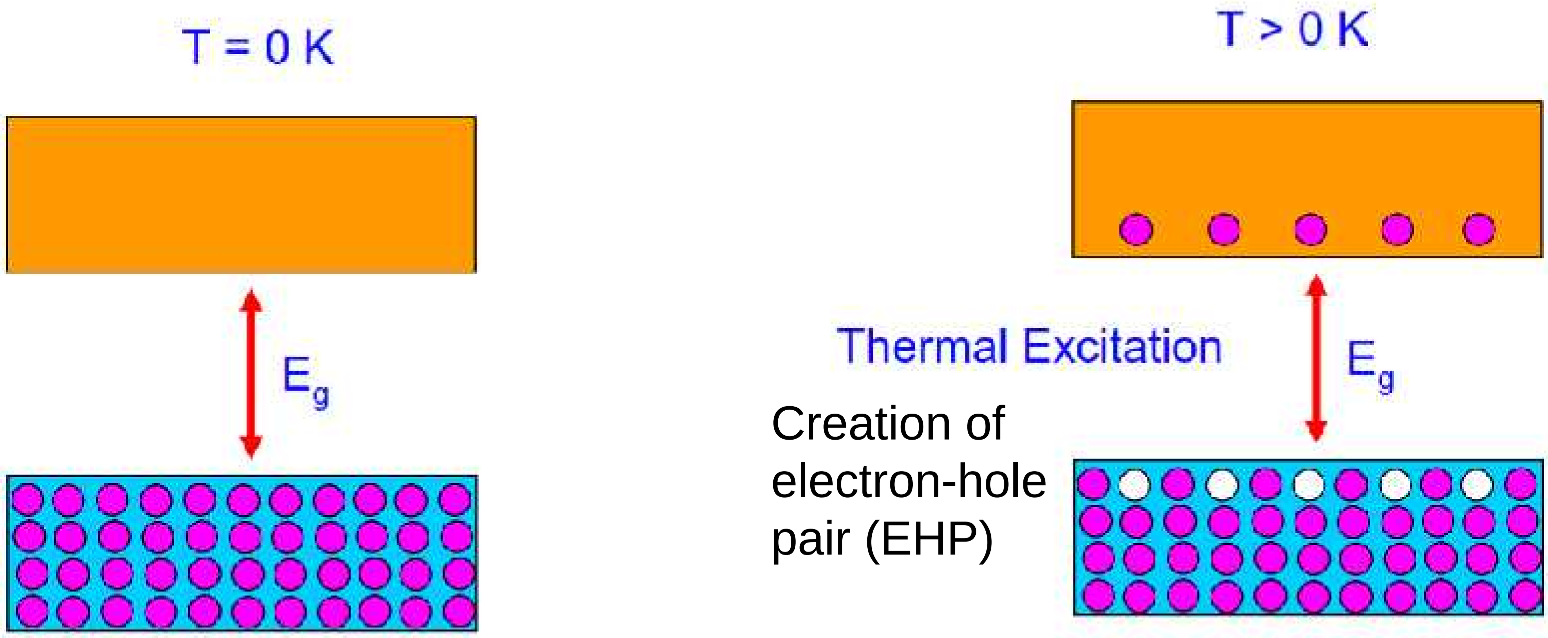


As x increase → all minimums moves up. But Γ minima moves up → E_g still direct until reaching x=0.38 → E_g becomes indirect

$x < 0.38$ $Al_xGa_{1-x}As$ is a direct semiconductor.
$x >= 0.38$ $Al_xGa_{1-x}As$ is an indirect semiconductor.

$x < 0.45$ $GaAs_{1-x}P_x$ is a direct semiconductor.
$x >= 0.45$ $GaAs_{1-x}P_x$ is an indirect semiconductor.

Electrons and Holes



Conduction Band: Empty
Valence Band: Filled
So, no conduction

Conduction band has electrons
Valence band has holes
So conduction by *both* electrons and holes

AN EMPTY CONDUCTION BAND OR A FILLED VALENCE BAND WILL NOT CONDUCT ELECTRICITY

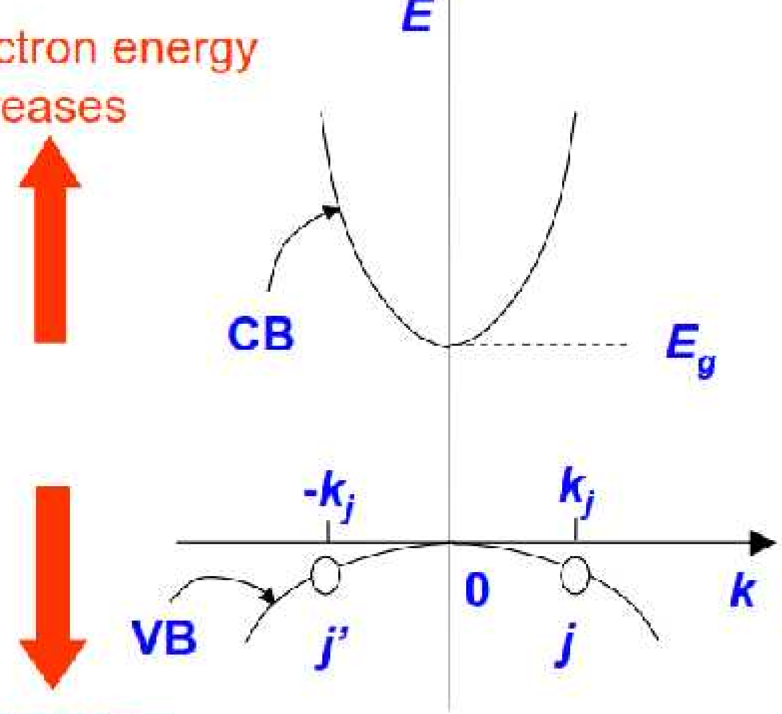
At T > 0^{o}K, electron are free to move in the C.B. full of empty states.
In the V.B., electrons move from hole to hole → holes appear to move

Electrons in Valence Band

Analogy: Water in a Bottle

Electrons: Water Droplets
Holes: Air bubbles

- Both empty bottle and filled bottle, when tilted, will not displace water.
- However, partially filled bottle when tilted, will allow movement of water.
- In valence band all states are filled (lowest energy level). Electron at j is matched by one at j' (hence no current flows unless one is removed By excitation into conduction band)



Electron energy increases

Hole energy increases

K=wave-vector in wave equation

- **Hole energy increases downward since holes have charges opposite to those of electrons. Primary reason why Holes are found in Valence Band (predominantly)**

Mathematical description

Conductivity due to hole: positively charged particle

Every j electron with velocity v_j have corresponding electron j’ with velocity $-v_j$ → current density

$$j = (-e)\sum_{i}^{N} v_i = 0$$

Net Current

for completely filled band, since electron occupation is symmetric in bands

$$j = (-e)\sum_{i}^{N} v_i - (-e)v_j = ev_j$$

for j^{th} hole (or missing electron).

In valence band, electron move from one hole to an other → hole appear to have a net motion → hole current

Note that the velocity (v_j) is governed by k, since k is the wave-vector in the wave equation:

$$\psi(x) = U(x)e^{i(kx-\omega t)}$$

Cell periodic function

Traveling part of wave-function

Hence, current flow in semiconductor is due to motion of charge carriers (electrons in the C.B. and holes in the V.B.)

Motion of Electrons in an Electric Field

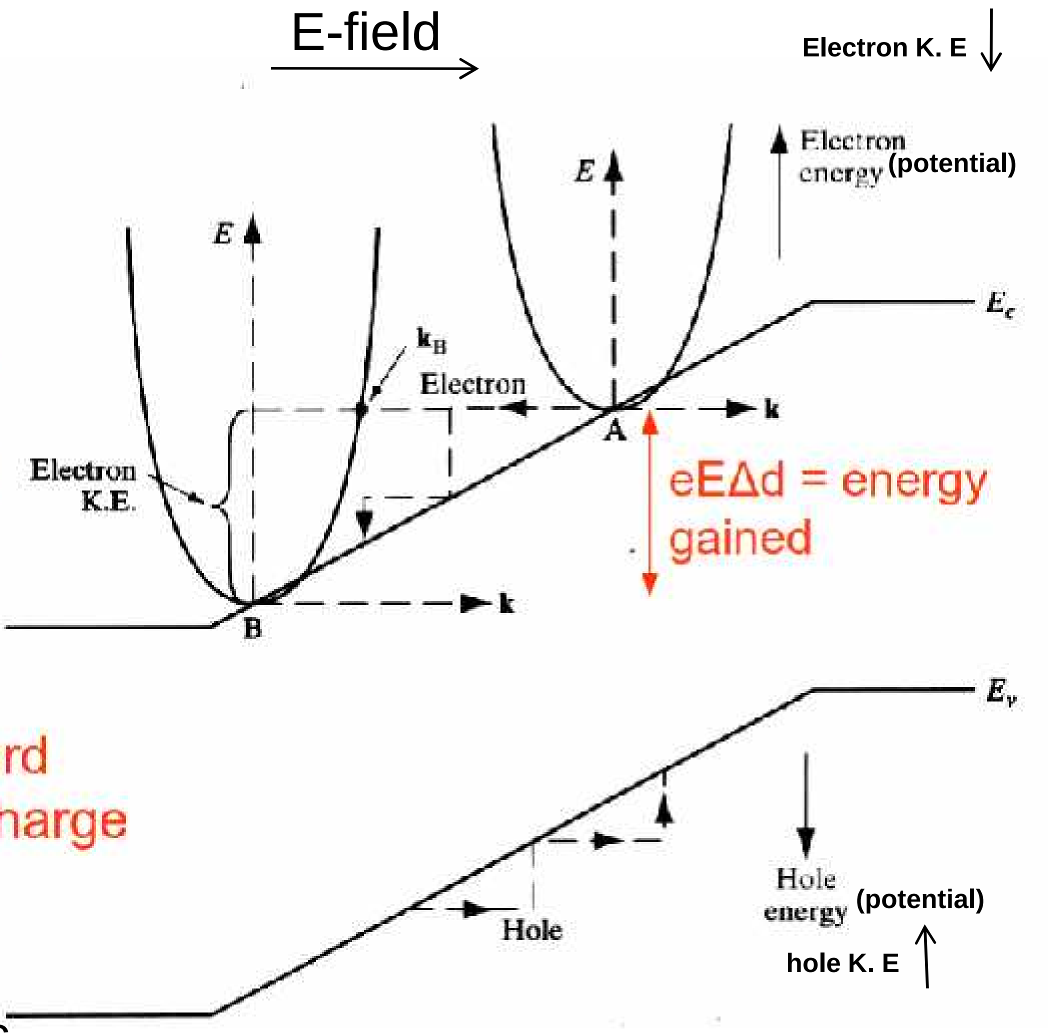
$$\Delta E_{Potential} = e\Delta V = eE\Delta d$$

Under an applied electric field the entire band structure shifts or equivalently the electron gains a kinetic energy of eEΔd

Electron will move from A to B gaining Kinetic energy and loosing potential energy

Hole energy increases downward since a hole has the opposite charge of an electron.

In valence band, Hole will move opposite to electron gaining Kinetic energy and loosing potential energy



eEΔd = energy gained

Under conservative force (Electric) electron will move opposite to E-field loosing potential energy and gaining kinetic energy. Hole will move with E-field loosing potential energy and gaining kinetic energy

Concept of Effective Mass (1)

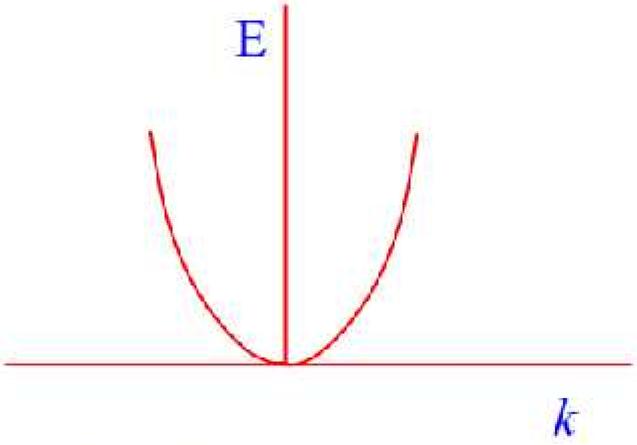
(a) Free Electrons (In the free space)

$$p = m\upsilon = \eta k$$ (de Broglie Wave)

$$E = \frac{m\upsilon^2}{2} = \frac{p^2}{2m} = \frac{\eta^2 k^2}{2m}$$

Note: η=h/2π

$$\Rightarrow \frac{d^2E}{dk^2} = \frac{\eta^2}{m} \Rightarrow \boxed{m = \frac{\eta^2}{d^2E/dk^2}}$$



Band for free electron

Meaning: **electron energy is parabolic. The mass is inversely related to the curvature of the parabola**

(b) Electrons in Solid : Electrons interact with the periodic potential of the crystal → they are not completely free

We would want to treat them in a similar way as that of free electrons

$$\frac{dp}{dt} = \frac{d(m\upsilon)}{dt} = F_{total} = F_{\text{int}} + F_{ext} \Rightarrow \frac{dp}{dt} = \frac{d\left(m^*\upsilon\right)}{dt} = F_{ext}$$ with $E = \frac{\eta^2 k^2}{2m^*}$

$$\Rightarrow \boxed{m^* = \frac{\eta^2}{d^2E/dk^2}}$$

Note: m* encapsulates the influence of lattice on the wave-particle behavior of the electron

**** Curvature of Band determines the effective mass**

Concept of Effective Mass (2)

So E-k diagram for electron inside semiconductor is given as: $E = \frac{\eta^2 k^2}{2m^*}$

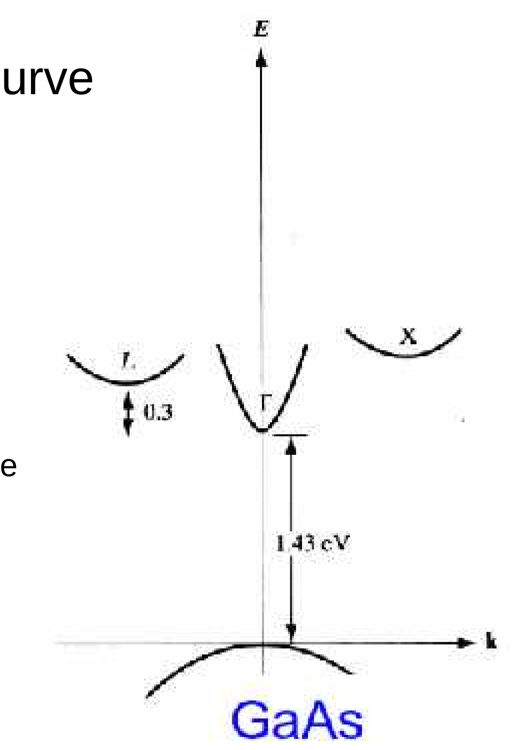
(c) Holes in Solid (Remember, holes are nothing but absence of electrons, so imagine movement of holes as movement of entire ensemble of electrons)

The curvature of d^2E/dk^2 is positive at the conduction band minima, but is negative at the valence band maxima. But considering that hole energy increases in the negative direction as electron energy, the hole mass is also positive at the valence band maxima.

NOTE: The effective mass is inversely proportional to the second derivative or curvature of the bands. Thus higher curvature or sharper bands will result in lower effective mass. So holes have higher effective mass than electrons

Concept of Effective Mass (2)

- hence,
- m^* is determined by the curvature of the E-k curve
- m^* is inversely proportional to the curvature



Some effective masses in solids

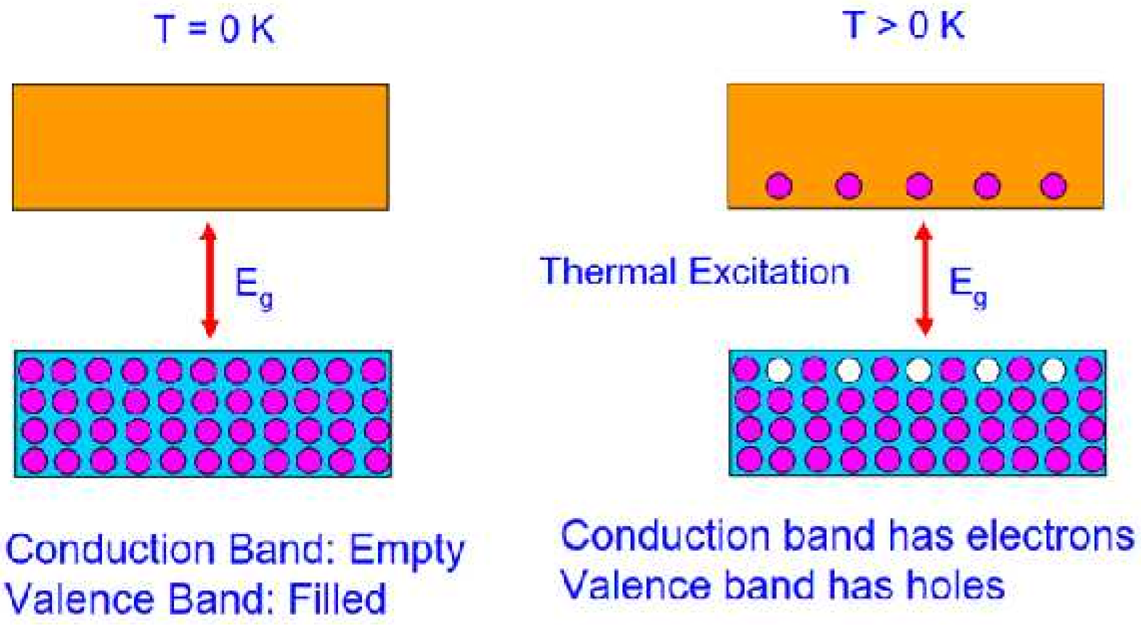
	Ge	Si	GaAs
m_n^*	0.55 m_e	1.08 m_e	0.067 m_e
m_p^*	0.37 m_h	0.56 m_h	0.45 m_h

m_n^* is the electron effective mass
m_p^* is the hole effective mass
m_e is the electron rest mass
m_h is the electron rest mass

* For GaAs band diagram, Γ has higher curvature than L and X → lower effective mass than in L and X.
* Highest effective mass will be found for hole at the valence band since it has lowest curvature

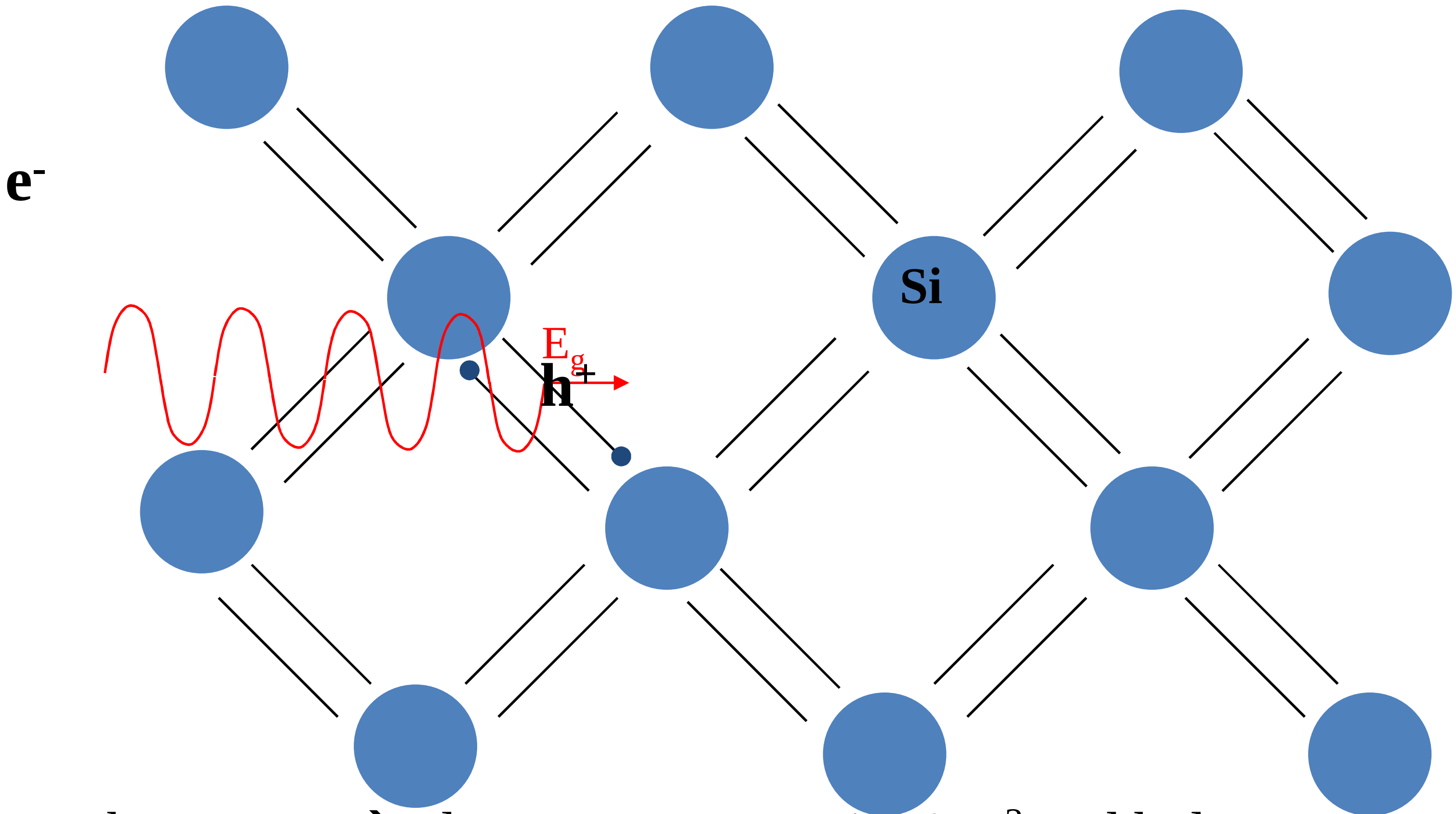
Intrinsic Material

- 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^{o}K, since the valence band is filled with electrons and the conduction band is empty.



Intrinsic Material

At T > 0 ºK → at Energy enough to broke the covalent bond → generation of electron hole pair (EHP); the only carriers in intrinsic semiconductor



Since we have EHP → electron concentration/cm^3 and hole concentration/cm^3 are equal and they are called intrinsic carrier concentration → $n = p = n_i$

Intrinsic Material

- If we denote the generation rate of EHPs as $g_i(EHP/cm^3s)$

and the recombination rate as $r_i(EHP/cm^3s)$

At given temperature, equilibrium requires that: $\boxed{r_i = g_i}$

Generation means creation of EHP and recombination means electron in C.B. make a transition to empty hole in the V.B.

Each of these rates is temperature dependent. For example,

$g_i(T)$ increases when the temperature is raised.

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

n_0 and p_0 are electrons and holes concentrations at equilibrium.

In intrinsic material the $n_0 = p_0 = n_i$ with

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

which is called the mass-action law

Extrinsic Material

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 semiconductors.

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*.

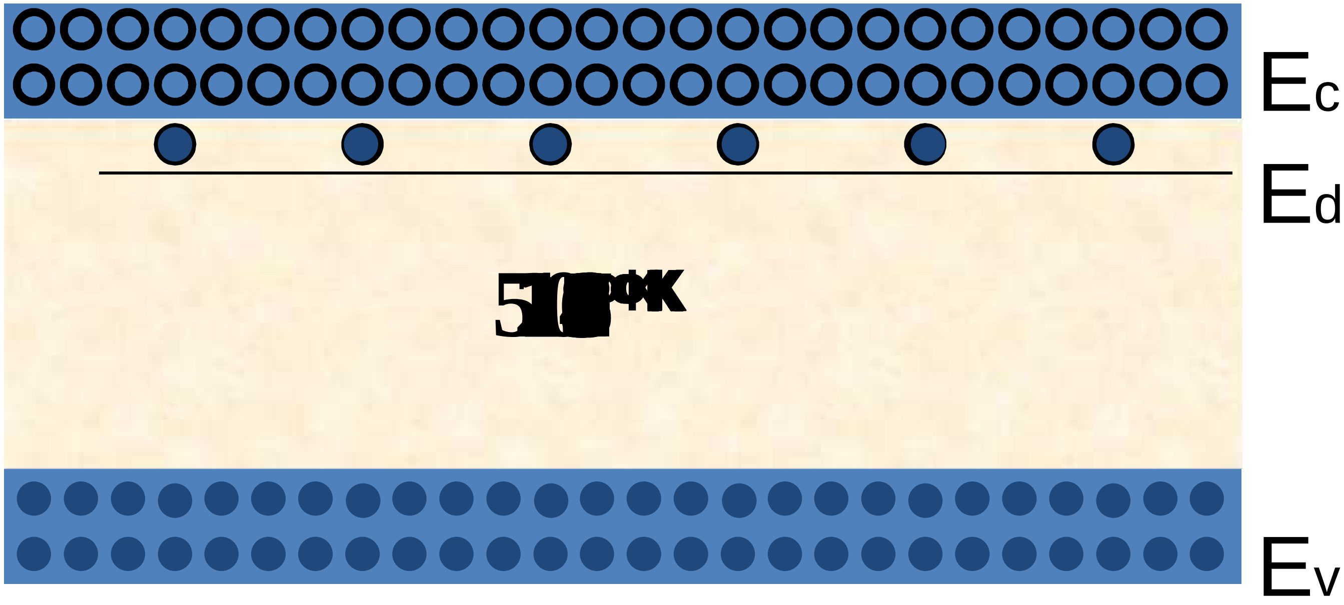
$$n_0 \neq p_0 \neq n_i \text{ but still } n_0 p_0 = n_i^2$$

n-type semicondutor: doping with impurity atoms from column V → donor atoms (gives extra electron in the conduction band) → majority electrons and minority holes

p-type semiconductor: doping with impurity atoms from column III → acceptor atoms atoms (takes electron from the valence band leaving holes behind) → majority holes and minority electrons

Extrinsic Material

V
P
As
Sb

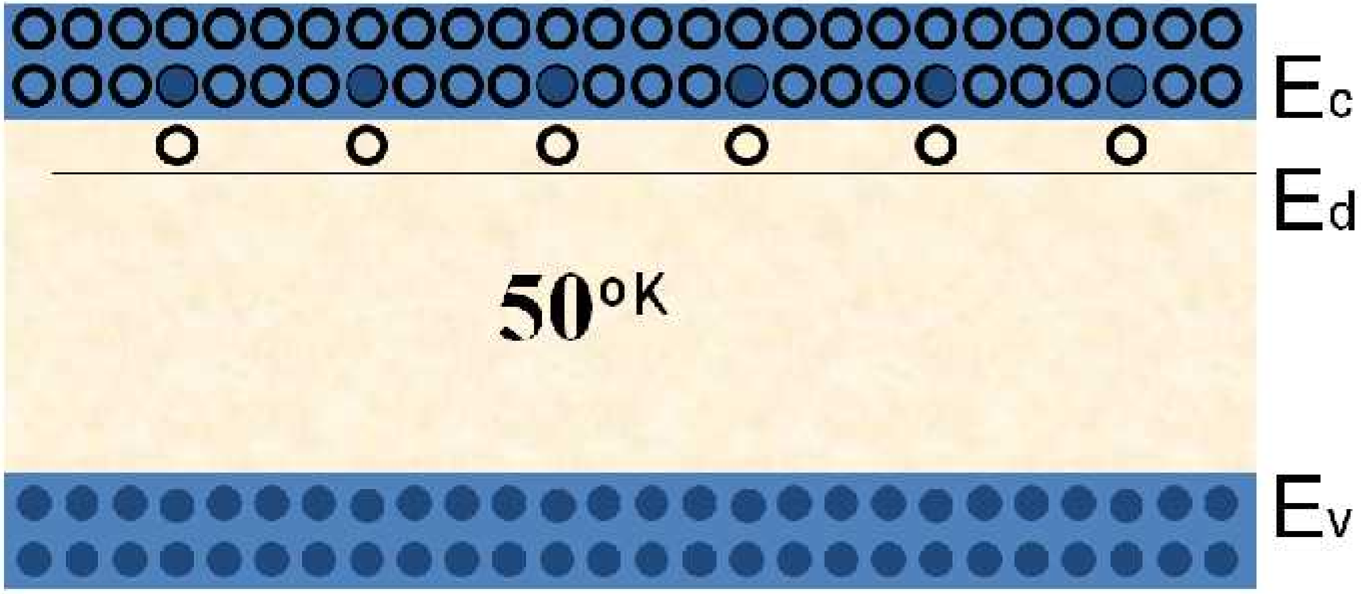


Donor

Extrinsic Material

Donor atoms introduce donor energy levels (E_d)near the conduction band so that the electrons exited to conduction band at low temperature (about 50 ºK)→ ($n_0>>p_0$ and $n_0>> n_i$)

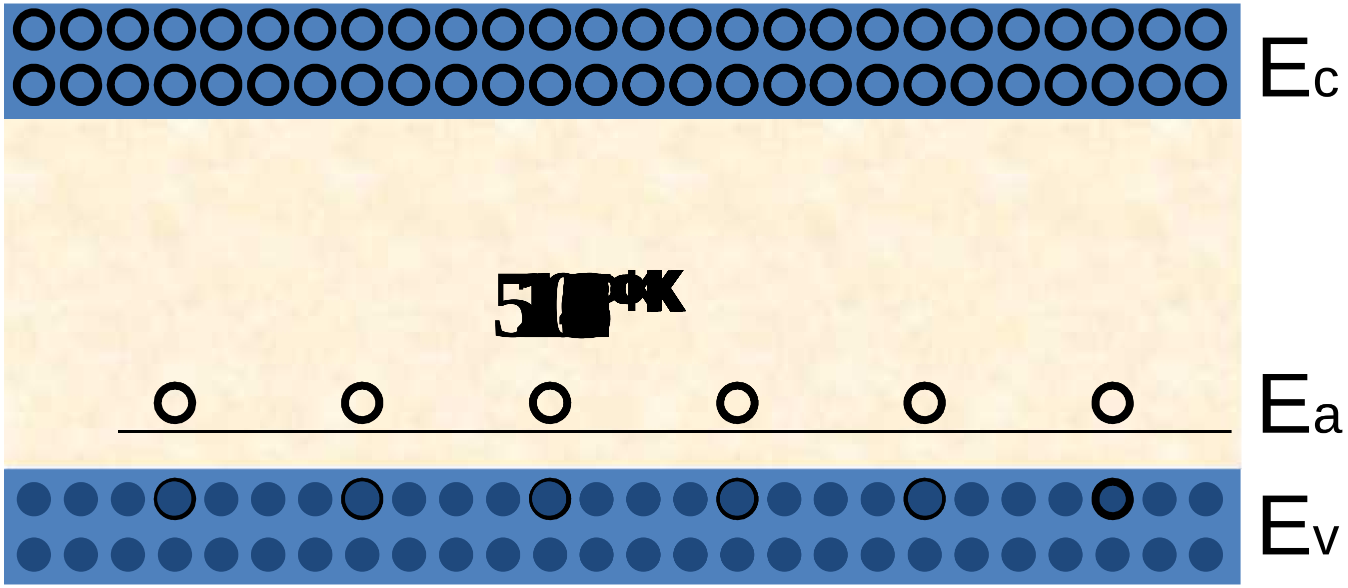
V
P
As
Sb



Donor

Extrinsic Material

III
B
Al
Ga
In

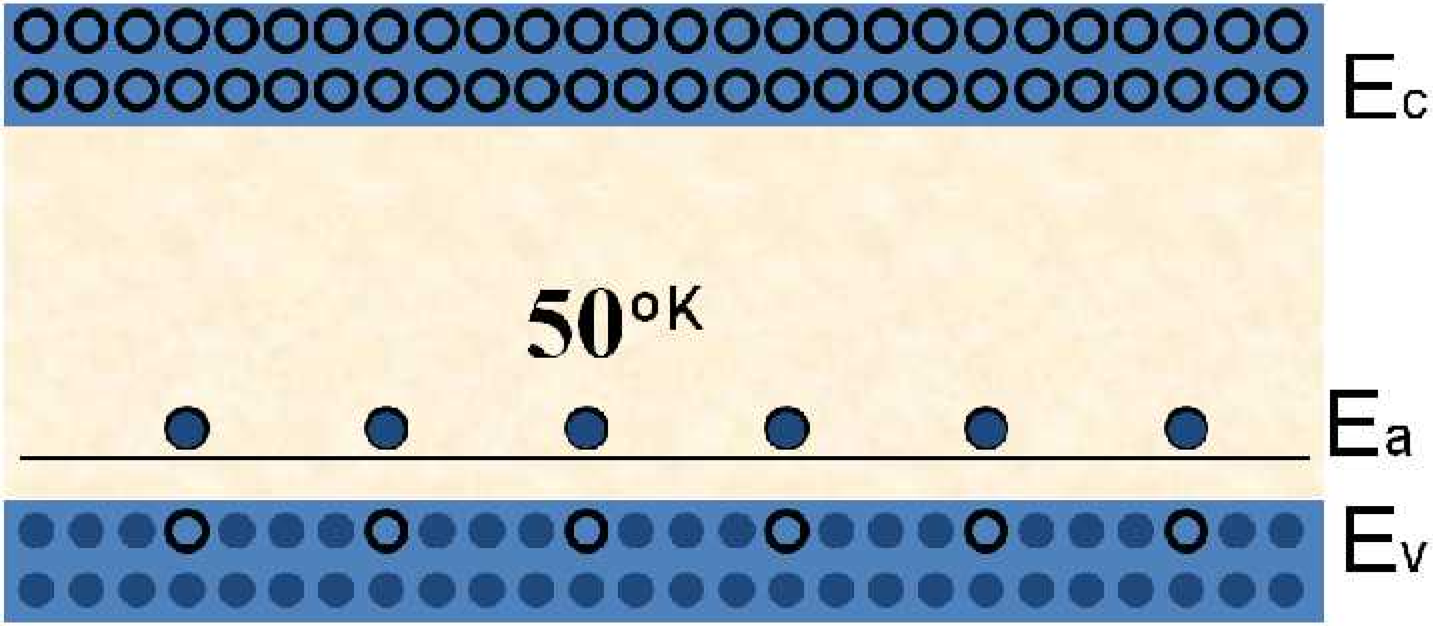


Acceptor

Extrinsic Material

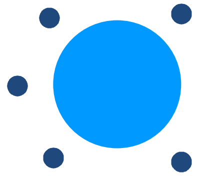
Acceptor atoms introduce acceptor energy levels (E_a) near the conduction band so that the electrons exited from valence band at low temperature (about 50 ºK) leaving holes behind ($p_0 >> n_0$ and $p_0 >> n_i$)

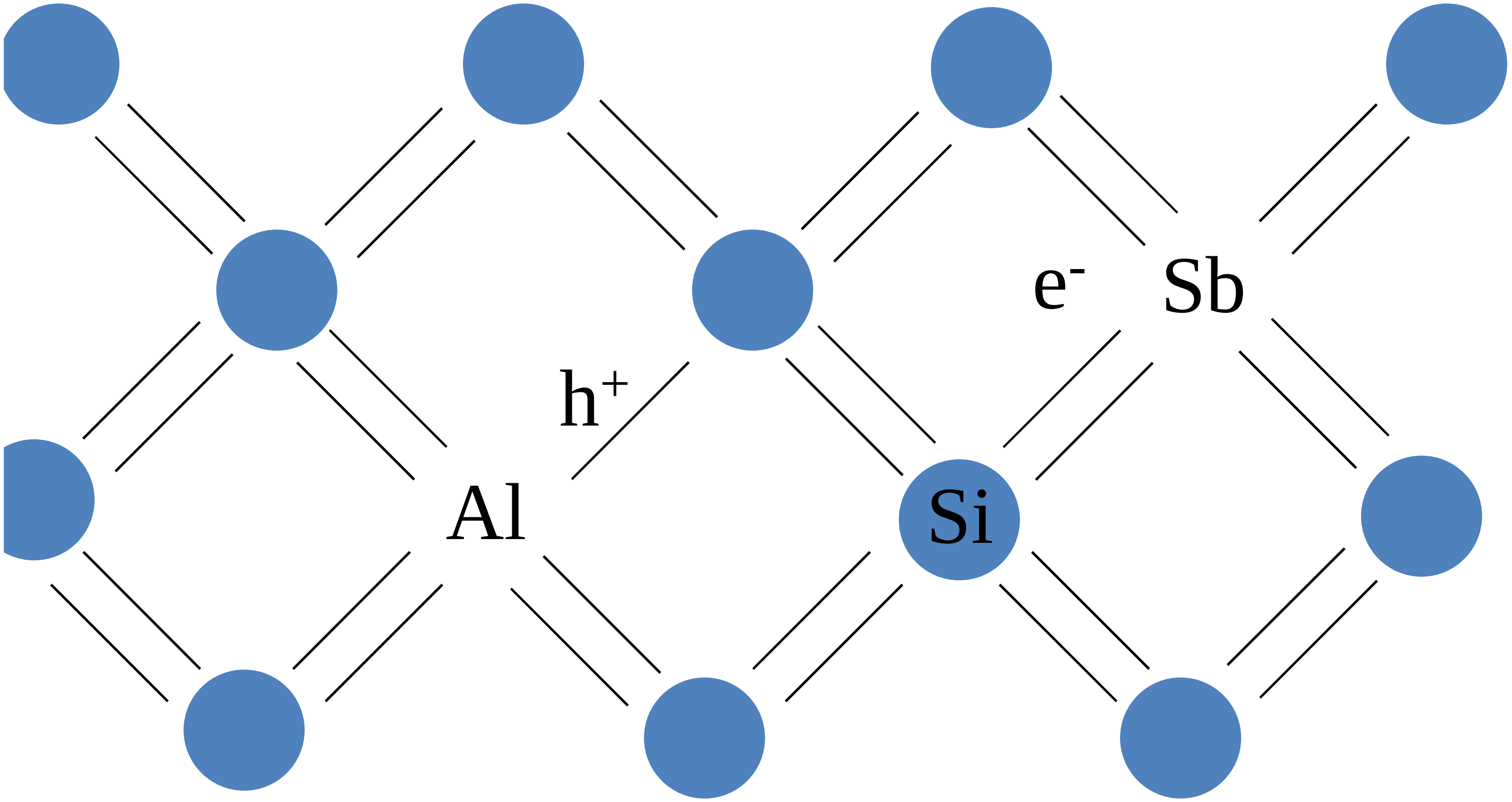
III
B
Al
Ga
In

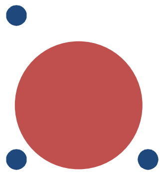


Acceptor

Extrinsic Material







Extrinsic Material

- We can calculate the *binding energy* by using the Bohr model results, consider-ing the loosely bound electron as ranging about the tightly bound “core” electrons in a hydrogen-like orbit.

$$E = \frac{mq^4}{2K^2\overline{h}^2}; n = 1, K = 4\text{®}\,\text{£}_0\text{£}_r$$

Extrinsic Material

- ❑ Example:

  Calculate the approximate donor binding energy for Ge($\varepsilon_{\boldsymbol{r}}$=16, $m_{\boldsymbol{n}}^{*}$=0.12$m_{\boldsymbol{0}}$).

- ❑ Answer:

$$E = \frac{m_n^* q^4}{8(\pounds_0 \pounds_r)^2 h^2}$$

$$= \frac{0.12(9.11\times10^{-31})(1.6\times10^{-19})^4}{8(8.85\times10^{-12}\times16)^2(6.63\times10^{-34})^2}$$

$$= 1.02\times10^{-21} J = 0.0064 eV$$

Thus the energy to excite the donor electron from n=1 state to the free state (n=∞) is ≈6meV.

Extrinsic Material

- Answer:

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Thus the energy to excite the donor electron from n=1 state to the free state (n=∞) is ≈6meV.

Carriers 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).
- Electrons in solids obey *Fermi-Dirac* statistics.

The concept of Fermi Level (1)

The Fermi-Dirac distribution gives the probability of occupancy of a state at a given temperature. Fermi level is analogous to the chemical potential

The Fermi level or Fermi energy is the energy, at which the probability of occupation by an electron (or hole) is exactly ½.

Fermi-Dirac Distribution Function:

$$\boxed{f(E)=\frac{1}{1+\exp[(E-E_F)/kT]}}$$

Things to note:

(a) Do not confuse this probability of occupancy in multiple electron system with the probability of finding a single electron in space.

(b) E_F denotes an energy level but does not imply that a state should be present at that energy level to be occupied.

(c) Physical significance of E_F is that it can be thought of as the mean of all the electron energy distribution.(where you will most likely find an electron)

DISTRIBUTION OF ELECTRONS IN SEMICONDUCTORS

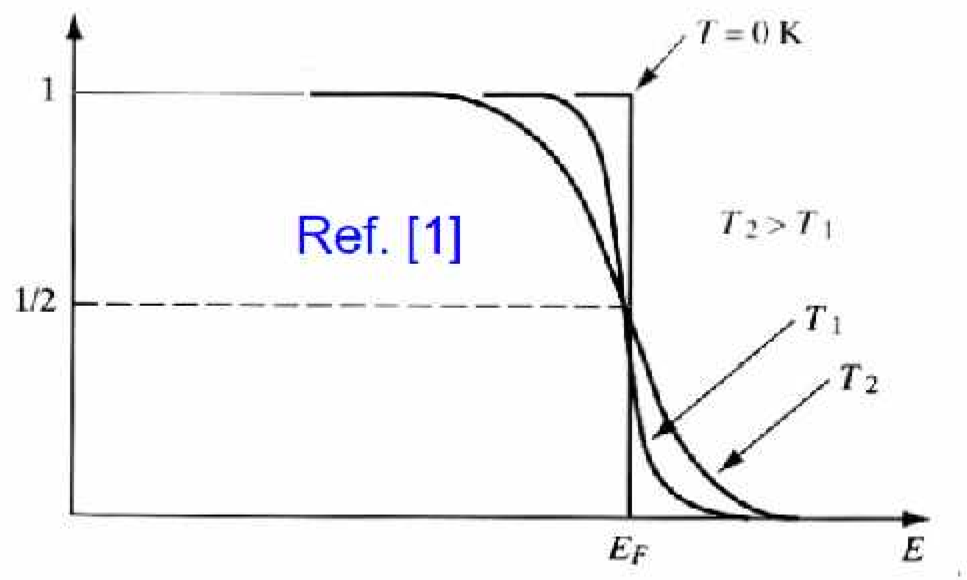
The Fermi Level (2)

The occupation probability at E = E_F,

$$f(E_F) = \frac{1}{1+\exp[(E_F - E_F)/kT]}$$

$$= \frac{1}{1+1} = \frac{1}{2}$$

- **T=0K,E<E_f f(E)=1/(1+0)=1 (all states occupied)**
- **T=0K, ,E>Ef f(E)=1/(1+∞) =0 (all above Ef are empty)**



Ref. [1]

Things to Note:

(1) The Fermi Function is symmetrical about E_F for all temperatures.

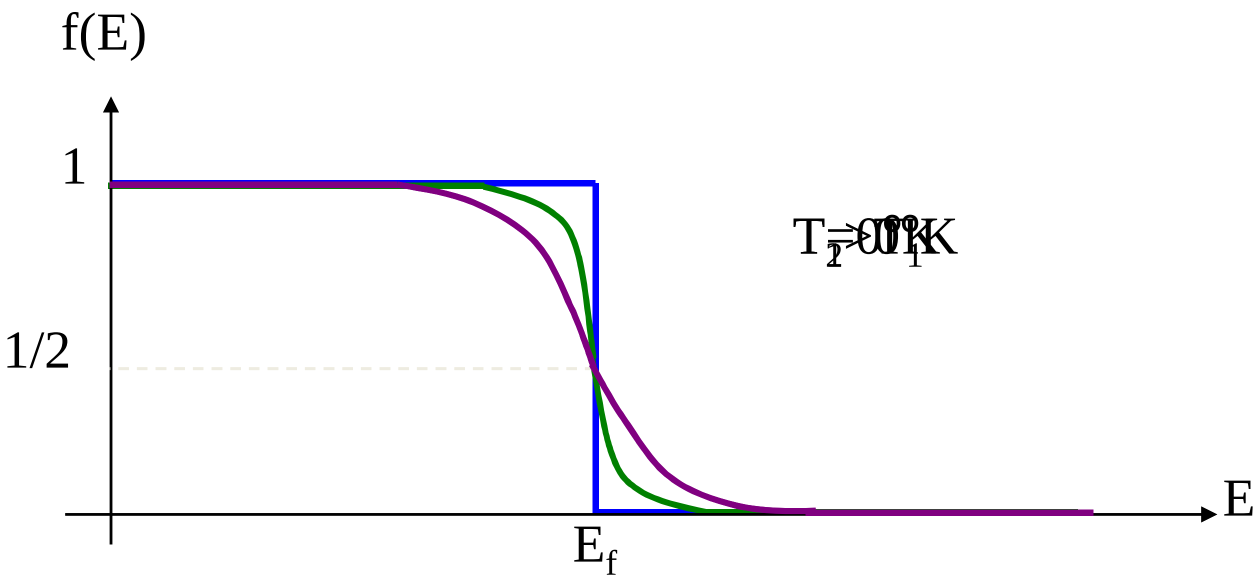
(2) At T = 0 K, this function has a simple rectangular form (binary occupational probability).

(3) At T = 0 K, available energy state up to E_F is filled with electrons, and all states above E_F are empty.

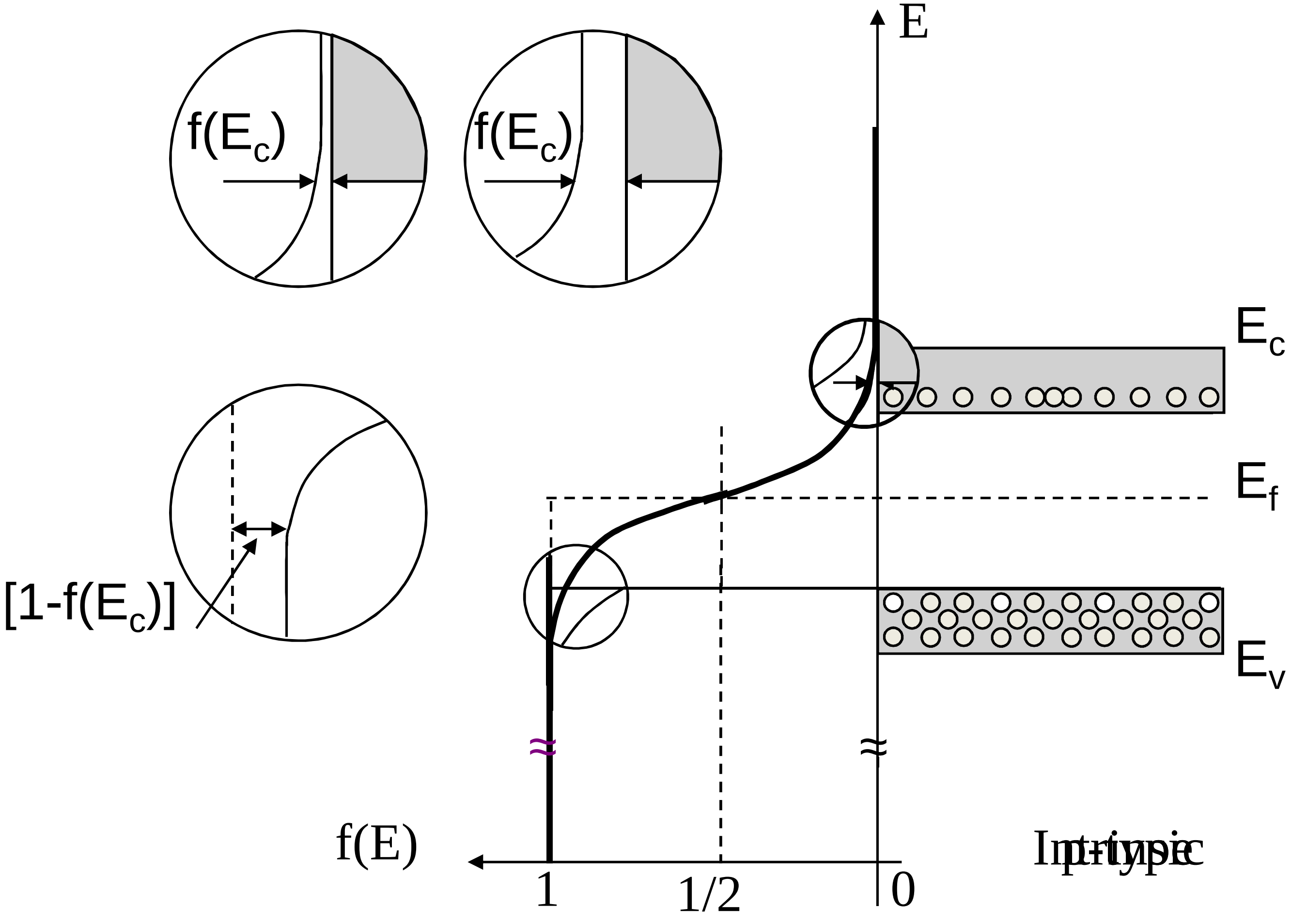
(4) It is not necessary that Fermi level is close to or superpose on energy states. In semiconductor, usually, Fermi level is in the band gap.

The Fermi Level

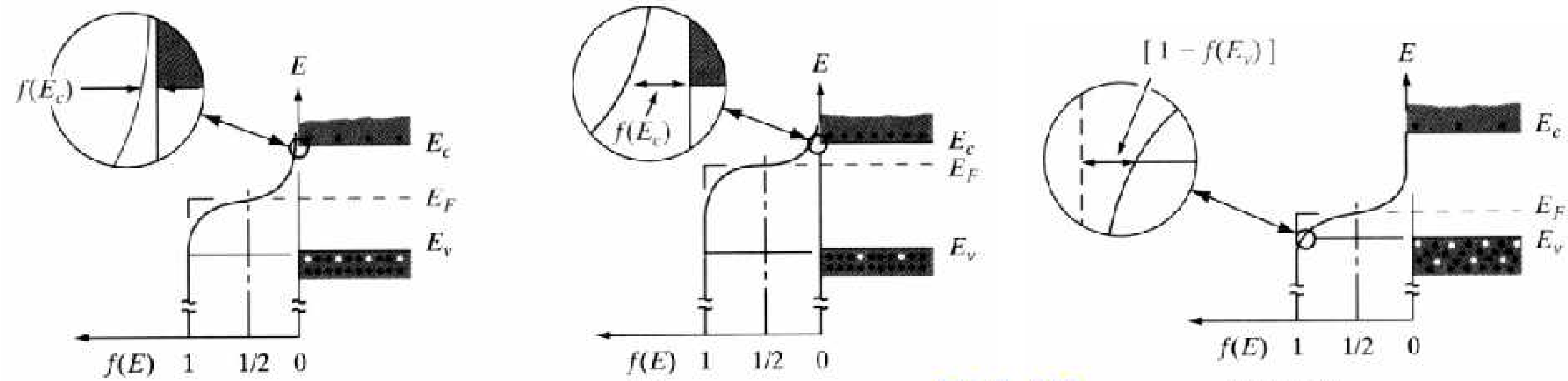
$$f(E_f) = \frac{1}{1+e^{(E_f - E_f)/kT}} = \frac{1}{1+1} = \frac{1}{2}$$



The Fermi Level



The Fermi Level (3)



(a) Intrinsic

$n_0 = p_0$

(b) n-type

Ref. [1]

(c) p-type

(1) In intrinsic material, the Fermi level is close to the middle of band gap.
(2) In n-type material, the Fermi level is close to the conduction band.
(3) In p-type material, the Fermi level is close to the valence band.

It is useful to think of Fermi level as a tool to determine electron/hole occupation at the conduction or valence band for a doped as well as undoped semiconductor in equilibrium.

Electron concentration in Conduction Band

$$n_0 = \int_{E_c}^{\infty} f(E)N(E)dE = N_C f(E_c) \qquad N(E) = \frac{\sqrt{2}}{\pi^2}\left(\frac{m^*}{\eta^2}\right)^{3/2} E^{1/2} \qquad \ldots\ldots\ldots\ldots \ (1)$$

(derivation in Appendix IV)

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

The Fermi function can be simplified for <u>many</u> (but not all) cases as:

$$f(E_C) = \frac{1}{1+\exp[(E_C - E_F)/kT]} \approx \exp[-(E_C - E_F)/kT]$$

[Valid only for $E_c - E_F >> kT$]

⇨ $$\boxed{n_0 = N_c \exp[-(E_c - E_F)/kT]} \qquad N_c = 2\left(\frac{2\pi m_n^* kT}{h^2}\right)^{3/2}$$

Remember the use of effective density of states N_c is very convenient, but does not bring out the real picture. N_c represents the <u>equivalent</u> density of states at the <u>conduction band edge (single energy level)</u>. Real density of states N(E) vary with energy, but effective density of states N_c does not

m_n^* is the density-of-states effective mass for electrons and is the geometric mean of the effective masses in the three directions.

Hole concentration in valence band

$$p_0 = N_v\left[1 - f\left(E_v\right)\right] \qquad N_v = 2\left(\frac{2\pi m_p^* kT}{h^2}\right)^{3/2} \qquad N\left(E\right) = \frac{\sqrt{2}}{\pi^2}\left(\frac{m^*}{\eta^2}\right)^{3/2} E^{1/2}$$

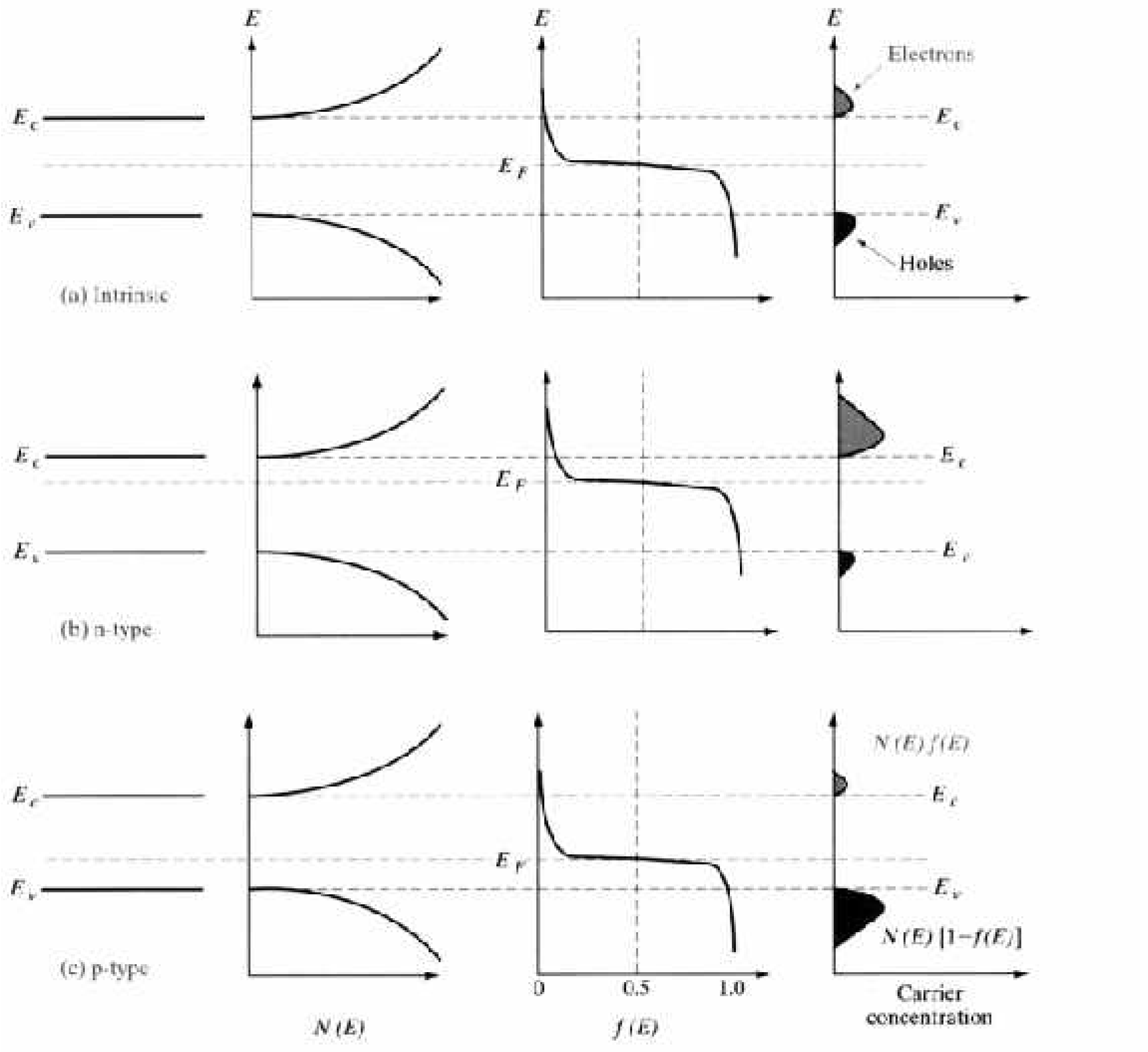
$$1 - f(E_v) = 1 - \frac{1}{1 + \exp[(E_v - E_F)/kT]} \approx \exp[-(E_F - E_v)/kT]$$

$$\Rightarrow \boxed{p_0 = N_v \exp[-(E_F - E_v)/kT]}$$

Effective density of states N$_v$ represents again the equivalent density of states (single energy) as opposed to as distribution of states as a function of energy.

m_p^* is the density-of-states effective mass for holes and is the geometric mean of the effective mass, similar to the electrons.

Fermi Level and electron distribution at Equilibrium



Fermi level at center indicates equal electron and hole distribution

Fermi level near CB indicates more electrons in CB than holes in VB

Fermi level near CB indicates less electrons in CB than holes in VB

Note: Here the real density of states an electron distribution has been shown

carrier density

For intrinsic semiconductors ($E_F = E_i$):

E_i is the intrinsic fermi energy level located at the middle of the energy gap

$$n_i = N_c \exp[-(E_c - E_i)/kT] \qquad p_i = N_v \exp[-(E_i - E_v)/kT]$$

$$n_i p_i = (N_c \exp[-(E_c - E_i)/kT])(N_v \exp[-(E_i - E_v)/kT])$$

$$= N_c N_v \exp(-E_g/kT) = n_i^2$$

Now, $n_i = p_i$ → $\boxed{n_i = \sqrt{N_c N_v} \exp(-E_g/2kT)}$ .... (2)

For extrinsic semiconductors ($E_F > E_i$, or $< E_i$):

$$n_0 p_0 = (N_c \exp[-(E_c - E_F)/kT])(N_v \exp[-(E_F - E_v)/kT])$$

$$= N_c N_v \exp[-(E_c - E_v)/kT]$$

$$= N_c N_v \exp(-E_g/kT)$$

→ $\boxed{n_0 p_0 = n_i^2}$ → $\boxed{\begin{aligned} n_0 &= n_i \exp[(E_F - E_i)/kT] \\ p_0 &= n_i \exp[(E_i - E_F)/kT] \end{aligned}}$

(Only valid under thermal equilibrium)

Electron and Hole Concentrations at Equilibrium

- Example 3-4:

  A Si sample is doped with 10^{17} As Atom/cm^3. What is the equilibrium hole concentration p_0 at 300°K? Where is E_F relative to E_i?

- Answer:

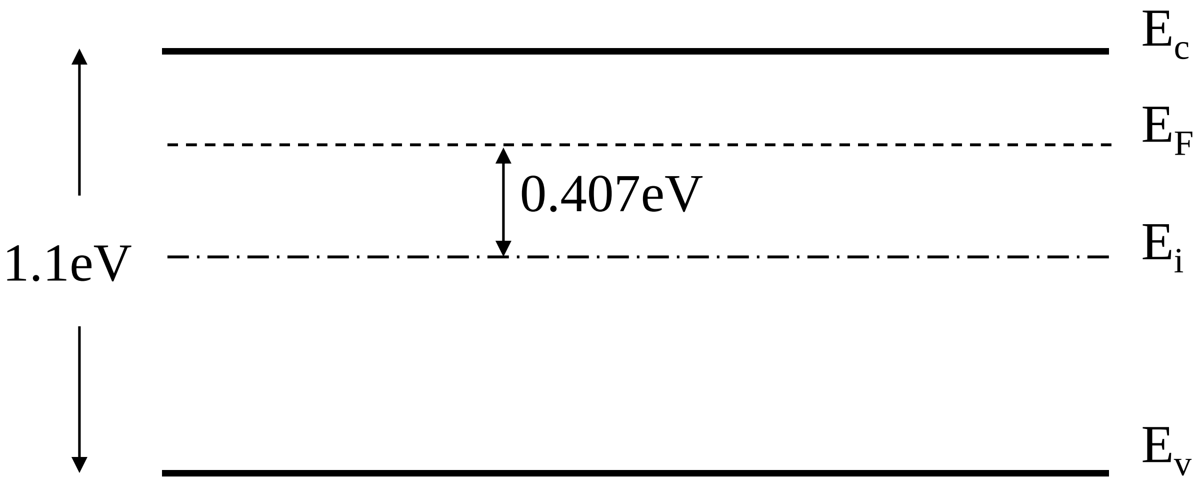
Since $N_d >> n_i$, we can approximate $n_0 = N_d$ and

$$p_0 = \frac{n_i^2}{n_0} = \frac{2.25\times10^{20}}{10^{17}} = 2.25\times10^{3}\,cm^{-3}$$

$$n_0 = n_i e^{(E_F-E_i)/kT} \quad \Longrightarrow \quad E_F - E_i = kT\ln\frac{n_0}{n_i} = 0.0259\ln\frac{10^{17}}{1.5\times10^{10}} = 0.407eV$$

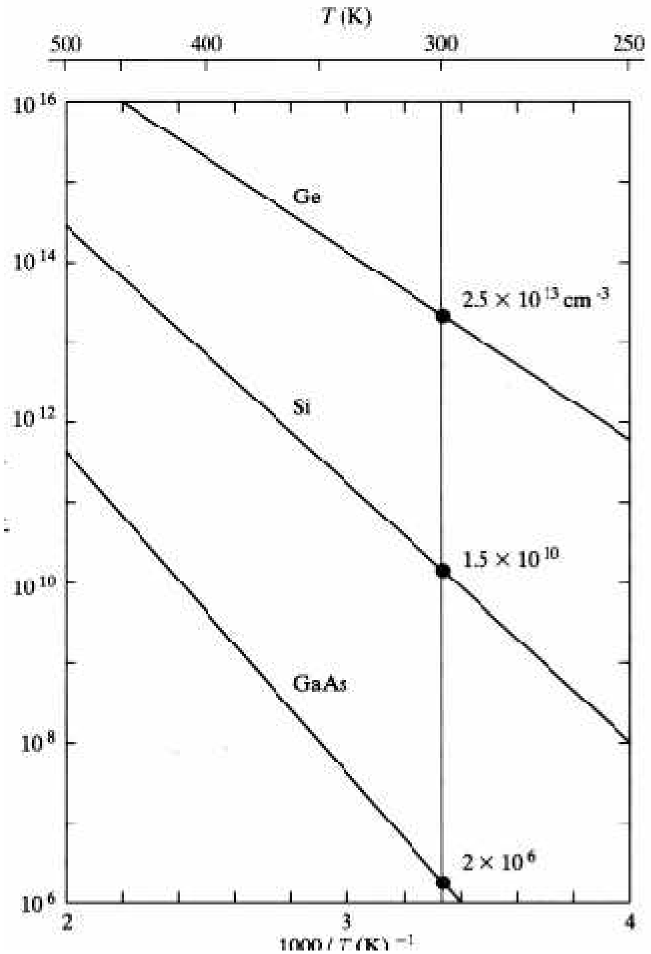
3-3-2. Electron and Hole Concentrations at Equilibrium

- Answer (Continue) :



Temperature vs. carrier concentrations

As for n_0 and p_0, n_i is also more temperature dependent and hence is E_F



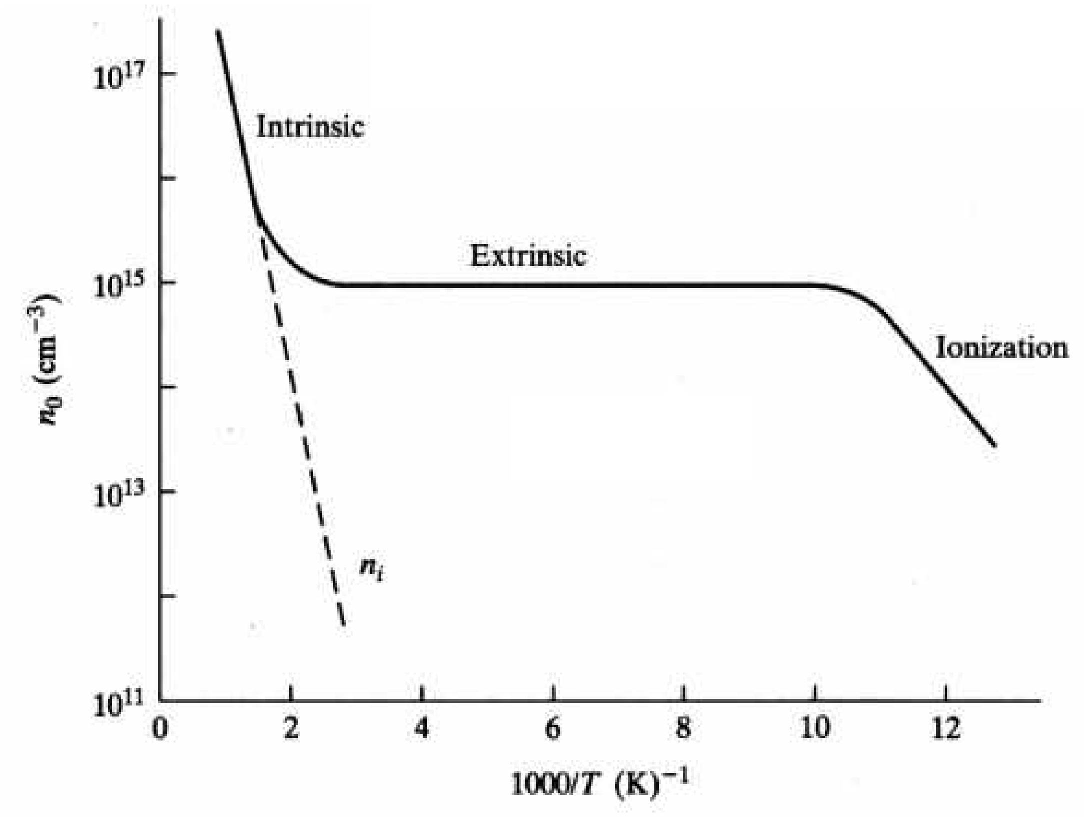
$$n_i = \sqrt{N_c N_v}\,\exp(-E_g / 2kT)$$

$$\boxed{n_i(T) = 2\left(\frac{2\pi kT}{h^2}\right)^{3/2} (m_n^* m_p^*)^{3/4} \exp(-E_g / 2kT)}$$

Note: The higher the bandgap, the lower the intrinsic carrier concentration

The dependence of carrier concentration in semiconductor on temperature passes into three regimes shown in the figure

Majority carrier concentration vs. inverse temperature for an extrinsic semiconductor. In the ionization regime, donor atoms are partially ionized. Then in the saturation regime where donors are fully ionized and carrier concentration is a constant. Finally, at high temperatures there is the intrinsic regime where it behaves like an intrinsic semiconductor. The temperatures corresponding to these depend on the donor concentration.



Compensation and Space Charge Neutrality

Space Charge Neutrality: In equilibrium every space inside a uniform semiconductor is *charge neutral*, or in mathematical terms

$$p_0 + N_d^+ = n_0 + N_a^-$$

For electrons in the conduction band:

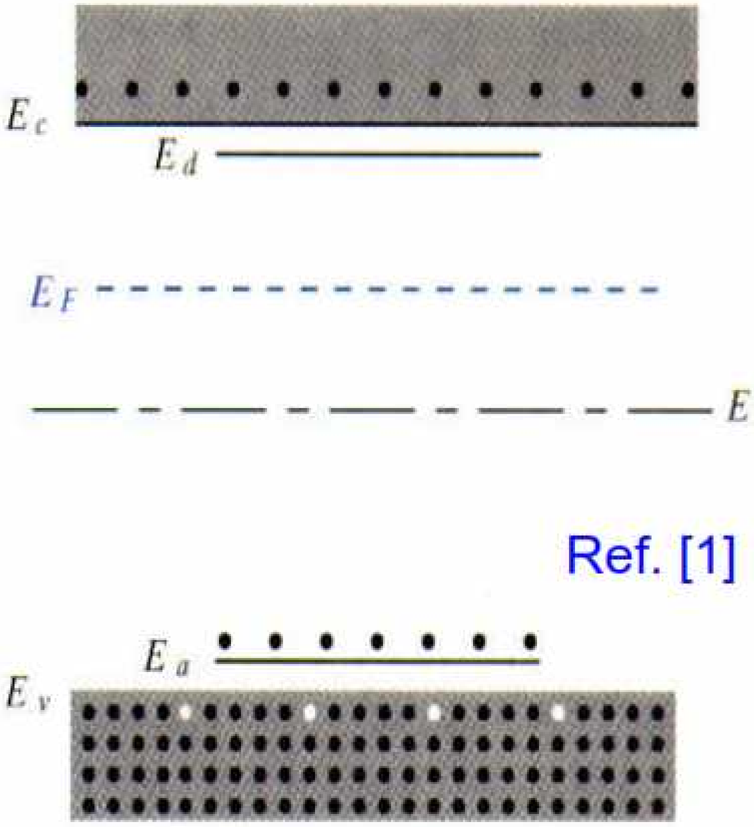
$$n_0 = p_0 + (N_d^+ - N_a^-)$$

If the material is n-type $n_0 >> p_0$, and all the impurities are ionized:

$$n_0 \approx N_d^+ - N_a^- \approx N_d - N_a$$

If the material is p-type $p_0 >> n_0$, and all the impurities are ionized:

$$p_0 \approx N_a^- - N_d^+ \approx N_a - N_d$$



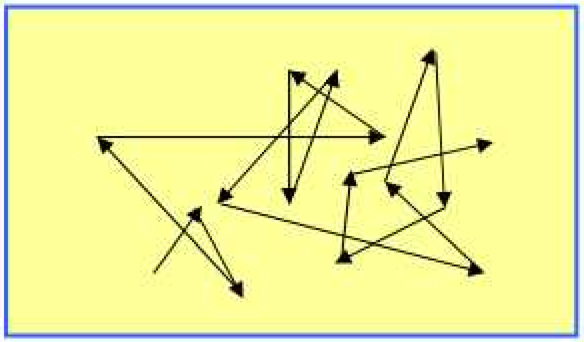
Ref. [1]

Note: As doping is increased slowly, the Fermi level moves toward the respective bands, and at some point may even penetrate the donor level and even the band.

Mobility (1)

(A) Motion of electrons and holes in solid at *thermal equilibrium*:

(1) Random thermal wandering
(2) Random scattering from the lattice and impurities
(3) No net motion of the group of N electrons, no preferred direction of motion
(4) An individual electron has a net motion, however, there is always another electron that has opposite net motion (reflected as k and –k state occupation in the E-k diagram.



Mobility represents the ease of electrons and holes to flow through the crystal under an externally applied electric field.

(B) Motion of electrons and holes in solid *in the presence of electric or magnetic fields.*

(1) Random thermal wandering + a net drift motion
(2) Random scattering from the lattice and impurities

Mobility (2)

In an external electric field, if electrons flow in a steady state, the net acceleration of electrons will be zero.

$$\frac{dp}{dt} = F_{tatol} = F_{ext} + F_{\text{int}} = 0 \quad F_{ext} = -nqE$$

***E* is the electric field**
Px = total momentum of carriers
N=# electrons/cm3
q=electronic charge

F_{int} is the retarding force, which comes from collision and scattering.

Collision rate: $-\frac{dN(t)}{dt} = \frac{1}{\tau_n} N(t)$

τ_n -represents the mean time between scattering events, is called mean free time or momentum relaxation time.

Mobility (3)

The probability that any electron has a collision in the time interval *dt* is

$$-\frac{dN(t)}{N(t)}=\frac{dt}{\tau_n} \Rightarrow$$

The differential change of momentum due to collisions is

$$dp_{collision}=-p\left(-\frac{dN(t)}{N(t)}\right)=-p\frac{dt}{\tau_n} \Rightarrow \left.\frac{dp}{dt}\right|_{collision}=-\frac{p}{\tau_n}=F_{\mathrm{int}}$$

$$\frac{dp}{dt}=F_{tatol}=F_{ext}+F_{\mathrm{int}}=0=-\frac{p}{\tau_n}-nqE$$

$\Rightarrow$ The average momentum per electron is $\boxed{\langle p\rangle=\frac{p}{n}=-q\tau_n E}$

$$\Rightarrow \boxed{\langle \upsilon\rangle=\frac{\langle p\rangle}{m_n^*}=-\frac{q\tau_n}{m_n^*}E=-\mu_n E}$$

Mobility (4)

The average momentum is proportional to the applied force, which is qE. The electrons, on an average, collide in time τ_n, so the momentum they achieve before reaching steady state is given as $q\tau_n E$

The average drift velocity <v> of electrons is then given as

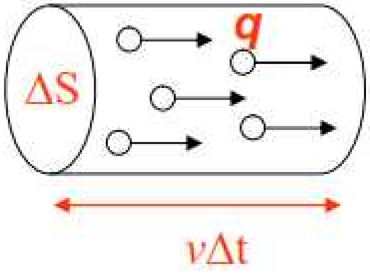
$$\boxed{\langle \upsilon \rangle = \frac{\langle p \rangle}{m_n^*} = -\frac{q\tau_n}{m_n^*}E = -\mu_n E}$$

m_n^* is the *conductivity effective mass* for electrons, which is the harmonic mean of the band structure effective masses. Note that this is different from the *density-of-states effective mass*, which is the geometric mean. μ_n is the electron mobility

Mobility (5)

(1) Current caused due to motion of <u>only</u> electrons in applied electric field:

$$j = \frac{\Delta Q}{\Delta S \cdot \Delta t} = \frac{qn\langle \upsilon \rangle \Delta t \Delta S}{\Delta S \Delta t}$$



$$j = qn\langle \upsilon \rangle = \frac{nq^2\tau_n}{m_n^*}E = nq\mu_n E$$

From Ohm's Law: $j = \sigma E$ $\Rightarrow$ $\sigma_n = \frac{nq^2\tau_n}{m_n^*} = qn\mu_n$ (only due to electrons)

(2) Total current due to <u>both</u> electrons and holes:

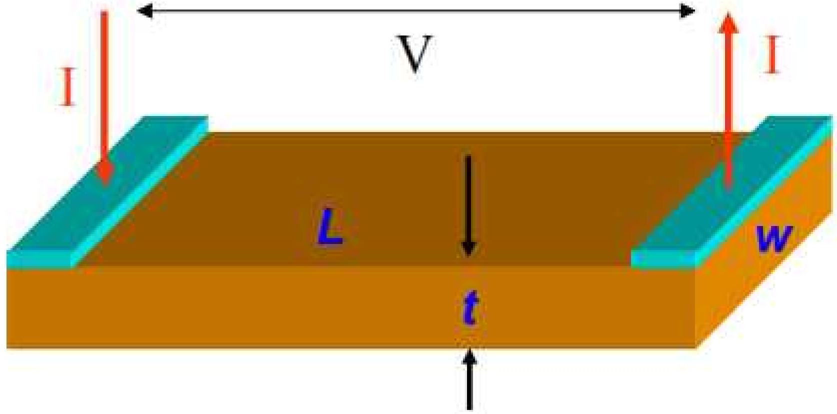
$$\boxed{j = qn\langle \upsilon_n \rangle + qp\langle \upsilon_p \rangle = \left(nq\mu_n + pq\mu_p\right)E = \sigma E}$$

$$\boxed{\sigma = qn\mu_n + qp\mu_p}$$

Note for holes, $\boxed{\langle \upsilon_p \rangle = \frac{q\tau_p}{m_p^*}E = \mu_p E}$

(μ_p is the hole mobility)

Resistance



$$R = \frac{V}{I} = \frac{\rho L}{wt} = \frac{L}{wt}\frac{1}{\sigma}$$

where $\sigma = qn\mu_n + qp\mu_p$

Tip: To calculate R first find σ from the electron and hole concentration, and then use the given dimensions of the sample

Note: Both the electrons and the holes take part in the conduction process

Example # 1

Problem: Calculate the resistivity of <u>intrinsic</u> Si at 300 K

Solution:

For intrinsic Si: $u_n = 1350$ and $u_p = 480$ cm^2/V-s from Appendix III.

Thus, since $n_0 = p_0 = n_i$

$$\sigma_i = q(\mu_n + \mu_p)n_i = 1.6\times10^{-19}(1830)\times1.5\times10^{10} = 4.39\times10^{-6}\ (\Omega.\mathrm{cm})^{-1}$$

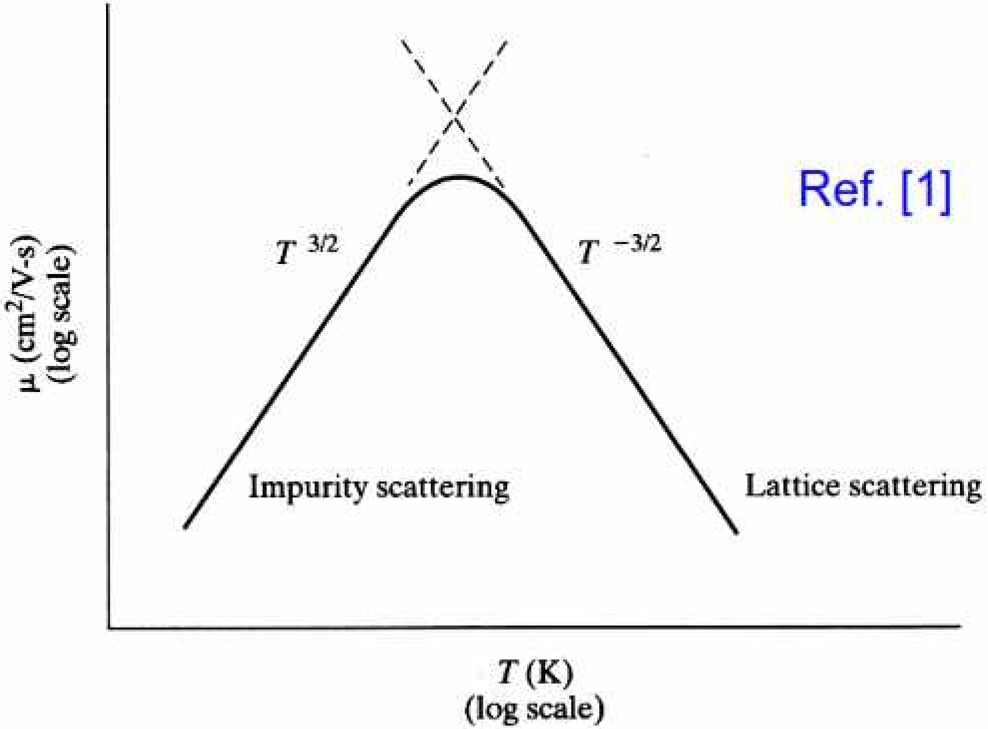
$$\rho_i = \frac{1}{\sigma_i} = 2.28\times10^{5}\ (\Omega.\mathrm{cm})$$

FACTORS AFFECTING MOBILITY

Effect of *Temperature* on Mobility

Two major scattering mechanisms:

1. Ionized impurity Scattering
2. Lattice Scattering or Phonon Scattering



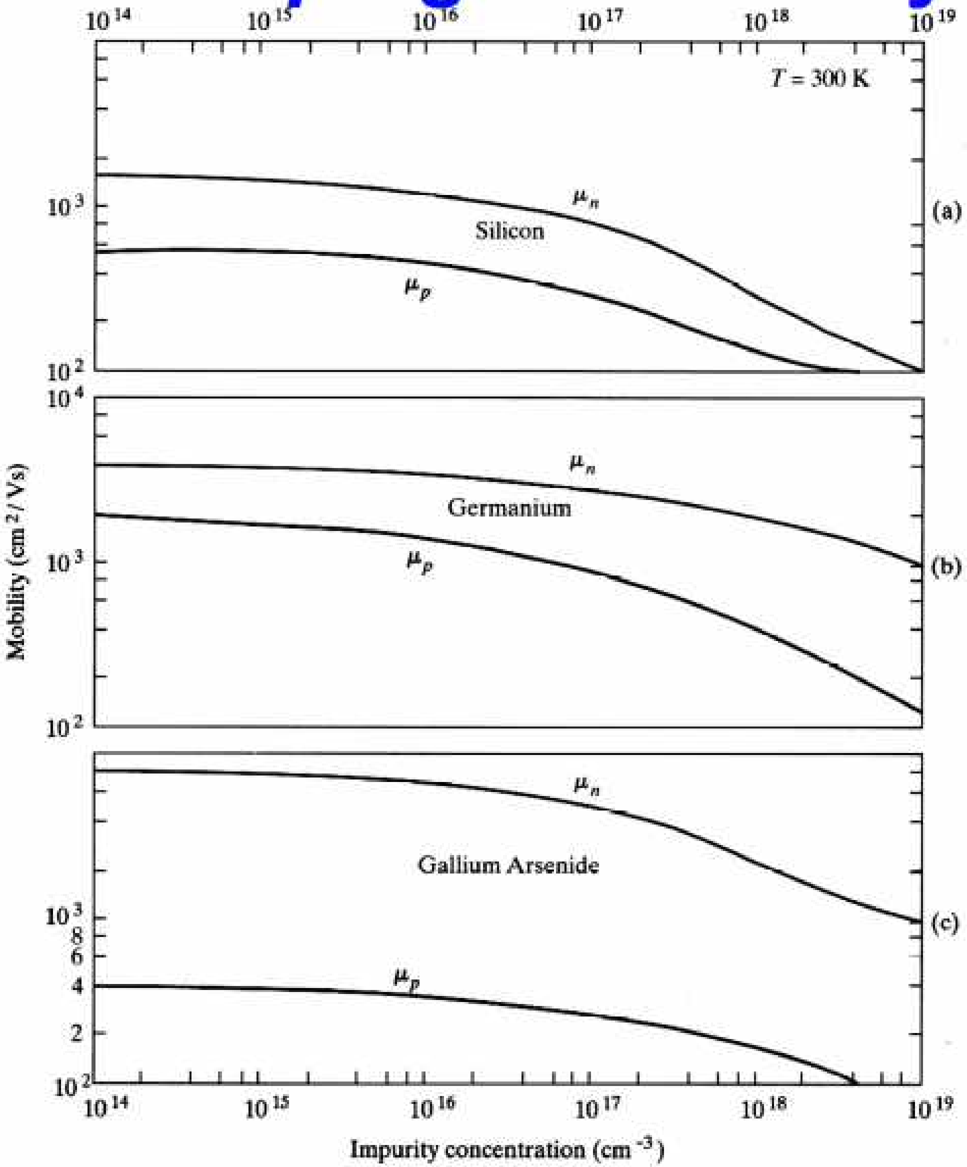
Ref. [1]

The overall mobility in presence of two or more independent scattering mechanisms is given by (Mattheisen's Rule):

$$\frac{1}{\mu} = \frac{1}{\mu_1} + \frac{1}{\mu_2} + \ldots$$

Effect of *Doping* on Mobility

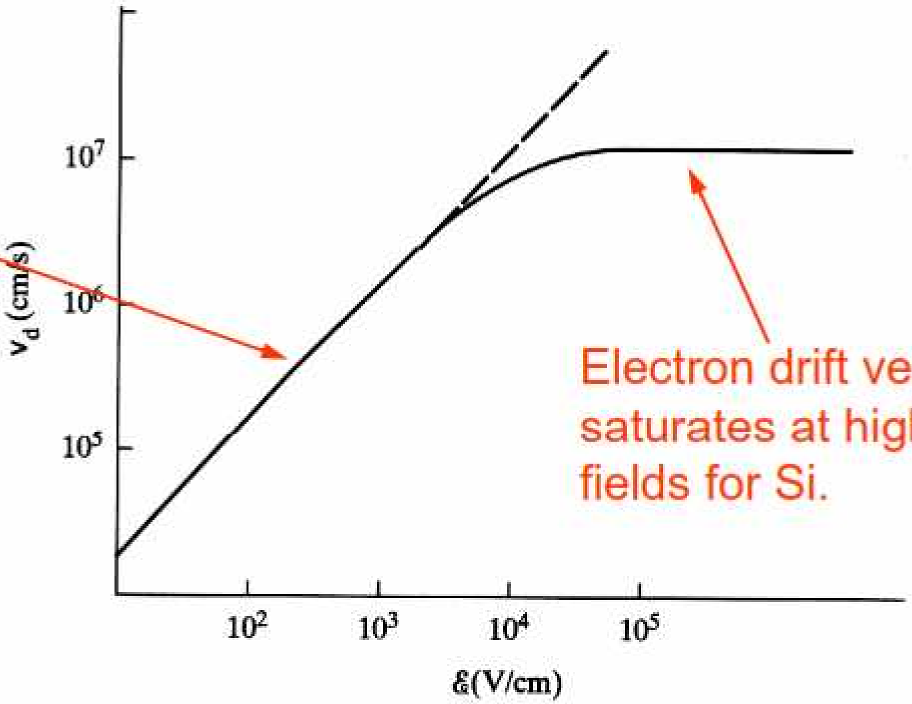
- The mobility reduces for higher doping due to increased ionized impurity scattering
- Compare the electron and hole mobility for Si, Ge, and GaAs



Ref. [1]

FACTORS AFFECTING MOBILITY

Effect of High-Field on Mobility



Slope gives the mobility only at <u>low</u> electric field

$$\langle \upsilon \rangle = -\mu_n E$$

is valid only at low field

Electron drift velocity saturates at high electric fields for Si.

Ref. [1]

1. At high electric field, the velocity of electrons CANNOT increase linearly with voltage due to increased scattering from the lattice vibrations (electron loses the entire extra energy from electric field immediately)
2. At a particular electric field called the <u>critical electric field</u>, the mobility becomes almost zero, and the velocity of the electrons become almost constant w.r.t. the electric field

The Hall Effect (1)

Hall effect is used to find mobility and carrier concentration in materials
The establishment of E-field E_y is called Hall-Effect

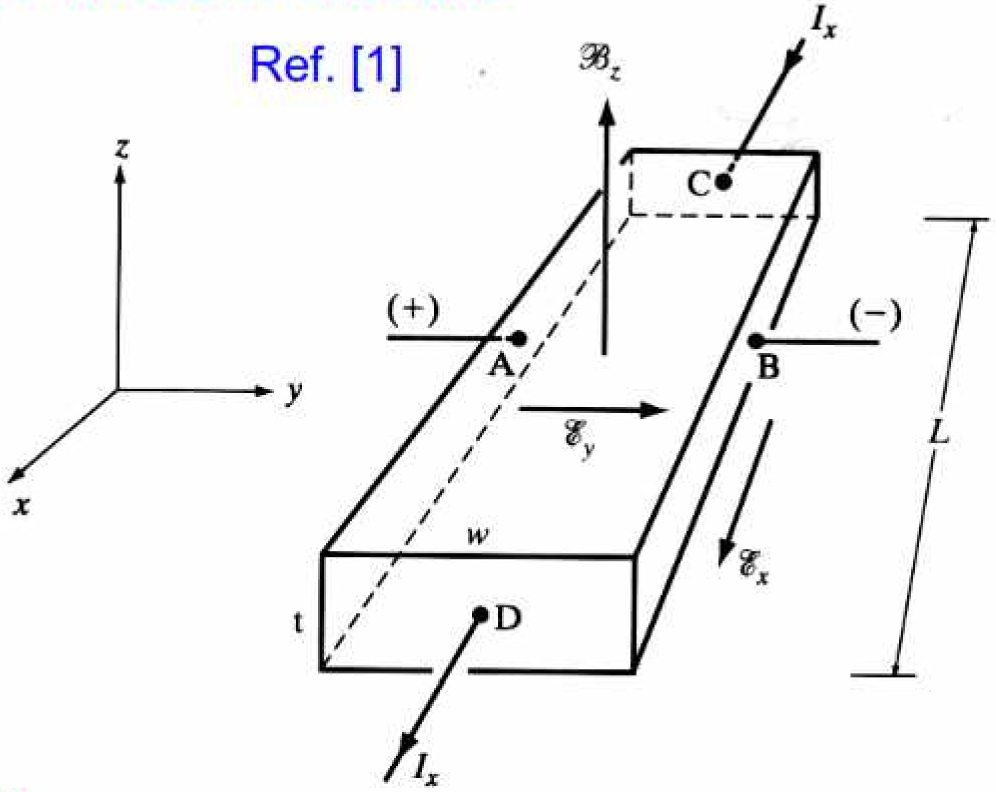
Experimental Observation:

If a constant current is flowing in x direction and magnetic Field is in z direction (perpendicular to holes direction), holes are deflected

then,

a voltage drop is built up in y or –y direction, depending on the charge (type) of carriers i.e. electrons or holes.

Ref. [1]



In equilibrium, the electric field built in y direction is generated to balance the magnetic field induced Lorentz force on the carriers.

The Hall Effect (2)

Lorentz Force (case considered for holes)

Force in y direction: $F_y = qE_y + q\upsilon_x \times B_z$ But we know, $F_y = 0$

➡ $E_y = \upsilon_x B_z$ ➡ $E_y = \dfrac{j_x}{qp_0} B_z = R_H j_x B_z$

Hall factor

$$\boxed{R_H = \frac{1}{qp_0}}$$

(positive for holes and negative for electrons)

➡ $$p_0 = \frac{1}{qR_H} = \frac{j_x B_z}{qE_y} = \frac{(I_x / wt) B_z}{q(V_{AB} / w)} = \frac{I_x B_z}{qtV_{AB}}$$

(Use to find doping)

Now for holes, $$\mu_p = \frac{\sigma}{qp_0} = \frac{1/\rho}{q(1/qR_H)} = \boxed{\frac{R_H}{\rho}}$$

(Use to find Mobility)

The Hall Effect (3)

If the carriers are electrons, then the Hall voltage $V_{AB\ (across\ Bar)}$ and Hall coefficient R_H are *negative*.

$$n_0 = \frac{1}{qR_H} = \frac{j_x B_z}{qE_y} = \frac{(I_x / wt)B_z}{q(V_{AB} / w)} = \frac{I_x B_z}{qtV_{AB}}$$

$$\mu_n = \frac{\sigma}{qn_0} = -\frac{1/\rho}{q(1/qR_H)} = \boxed{-\frac{R_H}{\rho}}$$

Thus, the sign of the *Hall voltage* can be used to determine the type of charge, and the magnitude can be used to calculate carrier density and mobility. Note sign of the Hall voltage is the same as the built in electric field E_y

Example # 3

Problem: A sample of Si is doped with 10^{17} phosphorus atoms/cm^3. What is the type of this semiconductor? What is the majority carrier concentration? What whould you expect to measure for its resistivity? What Hall voltage would you expect in a sample 100 μm thick if I_x = 1.0 mA and $\mathcal{B}_z = 1.0\mathbf{kG} = 10^{-5}\,\mathbf{Wb/cm^2}$?

Since phosphorus is element of the V th group its has 1 weakly bound electron in Si matrix. Thus, this is donor impurity and semiconductor is *n*-type. Since $N_d = 10^{17}\,\mathbf{cm}_{-3} << N_c$ Fermi energy should be sufficiently below E_c (i.e. $E_c - E_F >> kT = 0.0259$ eV and donor binding energy in Si). Thus almost all the donor levels will be ionized and electrons will occupy states in conduction band. As a result

$$n_0 \approx N_d$$

From Fig. 3-23 of the textbook, the mobility of electrons is 700 cm^2/(Vs). Thus the conductivity is (p_0 is negligible)

$$\sigma = q\mu_n n_0 = 1.6 \cdot 10^{-19} \cdot 700 \cdot 10^{17} = 11.2(\Omega \cdot \mathbf{cm})^{-1}.$$

The resistivity is

$$\rho = 1/\sigma = 0.0893\Omega \cdot \mathbf{cm}\,.$$

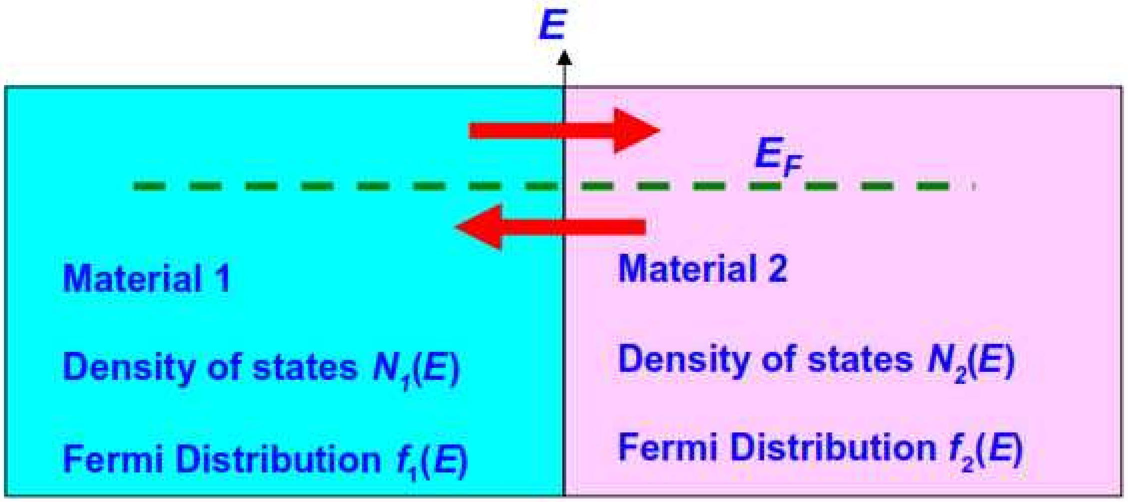
From (11-9), the Hall coefficient is

$$R_H = -(qn_0)^{-1} = -62.5\mathbf{cm}^3/\mathbf{C}\,.$$

The Hall voltage is

$$V_{AB} = \frac{I_x \mathcal{B}_z}{t} R_H = \frac{10^{-3}\,\mathbf{A} \cdot 10^{-5}\,\mathbf{Wb/cm}^2}{10^{-2}\,\mathbf{cm}} \cdot (-62.5\mathbf{cm}^3/\mathbf{C}) = -62.5\,\mu\mathbf{V}$$

Invariance of the Fermi Level at Equilibrium



E

E_F

Material 1

Density of states $N_1(E)$

Fermi Distribution $f_1(E)$

Material 2

Density of states $N_2(E)$

Fermi Distribution $f_2(E)$

Rate of charge movement from 1 to 2 $\propto N_1(E) f_1(E) \cdot N_2(E)[1 - f_2(E)]$

Rate of charge movement from 2 to 1 $\propto N_2(E) f_2(E) \cdot N_1(E)[1 - f_1(E)]$

At equilibrium both rates are equal (since no net movement of charge):

$$N_1(E) f_1(E) \cdot N_2(E)[1 - f_2(E)] = N_2(E) f_2(E) \cdot N_1(E)[1 - f_1(E)]$$

➡ $\boldsymbol{f_1(E) = f_2(E)}$ So, in the limit of the regions very small $\boxed{\frac{dE_F}{dx} = 0}$

Message:

In equilibrium Fermi level E_F is same everywhere (zero gradient)