Semiconductor Materials

Semiconductor Band theory and Formation allowed and forbidden band

Second stage: General Science
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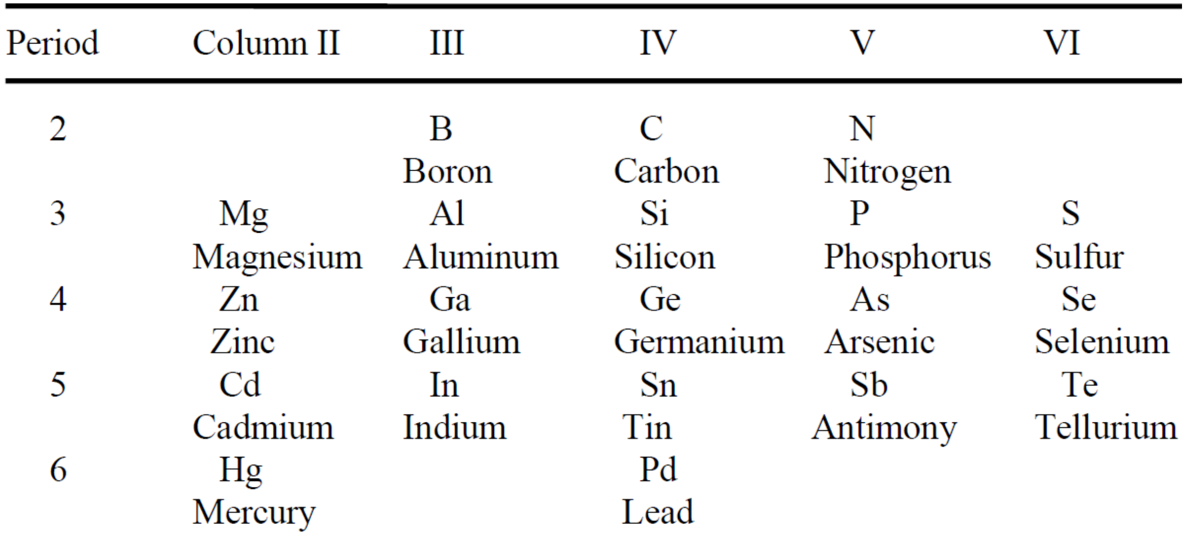
Type of Semiconductors according to their structure

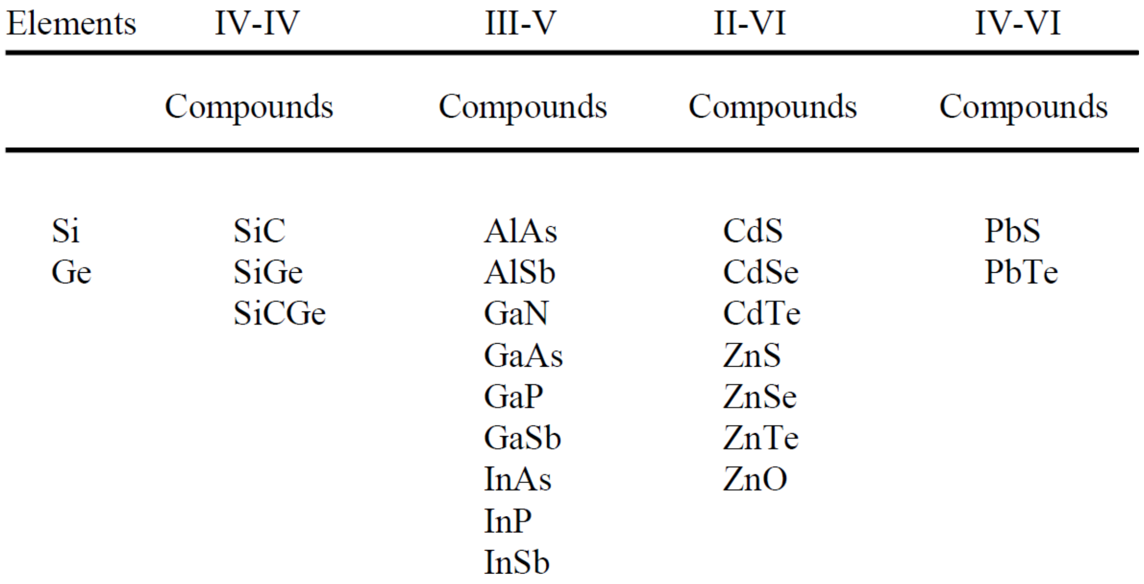
Semiconductors can be composed of a single element such as silicon and germanium or consist of two or more elements for compound semiconductors. A binary III-V semiconductor is one comprising one element from Column III (such as gallium) and another element from Column V (for instance, arsenic). The common element and compound semiconductors are displayed in Table

Portion of the Periodic Table Related to Semiconductors



Period	Column II	III	IV	V	VI
2		B Boron	C Carbon	N Nitrogen	
3	Mg Magnesium	Al Aluminum	Si Silicon	P Phosphorus	S Sulfur
4	Zn Zinc	Ga Gallium	Ge Germanium	As Arsenic	Se Selenium
5	Cd Cadmium	In Indium	Sn Tin	Sb Antimony	Te Tellurium
6	Hg Mercury		Pd Lead		

Element and compound semiconductors



Elements	IV-IV	III-V	II-VI	IV-VI
	Compounds	Compounds	Compounds	Compounds
Si	SiC	AlAs	CdS	PbS
Ge	SiGe	AlSb	CdSe	PbTe
	SiCGe	GaN	CdTe	
		GaAs	ZnS	
		GaP	ZnSe	
		GaSb	ZnTe	
		InAs	ZnO	
		InP		
		InSb		

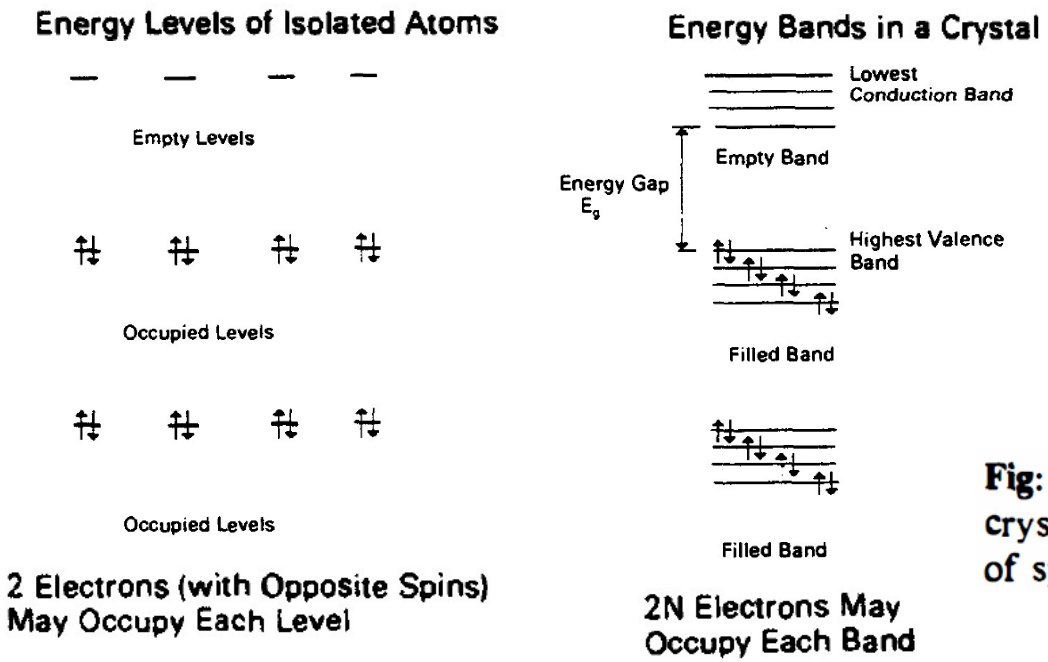
Formation of bands in solid

Consider again regular period arrangement of atom, in which each atom now contain more than one electron .suppose the atom in this imaginary crystal contains electrons up through the $n = 3$ *energy levels*

If the atoms are initially very far apart, the electrons in adjacent atoms will not interact and will occupy the discrete energy levels. If these atoms are brought closer together, the outermost electrons in the $n = 3$ *energy levels* will begin to interact initially, so that this discrete energy level will split into a band of allowed energies.

If the atoms continue to move closer together, the electrons in the $n = 2$ *energy level* may begin to interact and will also discrete energy levels split into a band of allowed energies. Finally, if the atoms become sufficiently close together, the innermost electrons in then $n = 1$ *energy level* level may interact so that this energy level may also split into a band of allowed energies. The splitting of these discrete energy levels is shown in figure below

Figure : Schematic showing the splitting **of** three energy states into allowed bands of energies



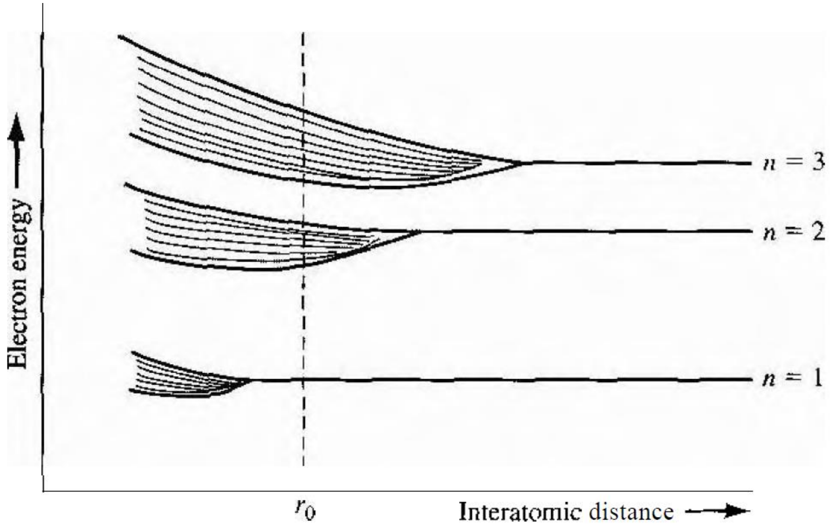
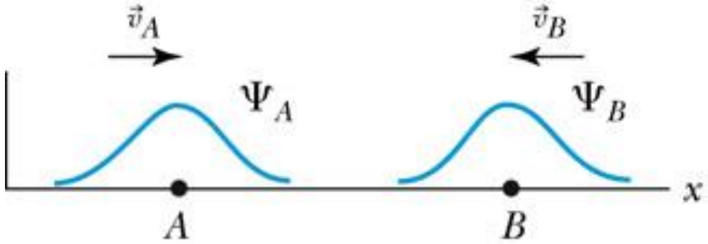


Fig: Splitting of energy levels of isolated atoms into energy bands in a crystal. Arrows pointing up and down represent electrons with different values of spin ($S = \pm\frac{1}{2}$).

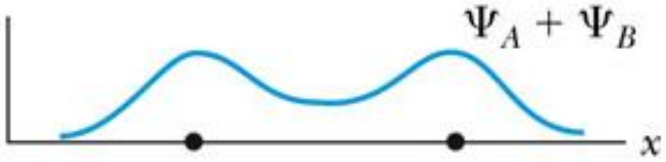
Band Theory of Solids

- **In order to account for *decreasing* resistivity with increasing temperature as well as other properties of semiconductors, a new theory known as the band theory is introduced**.
- **The essential feature of the band theory is that the allowed energy states for electrons are nearly continuous over certain ranges, called energy bands, with forbidden energy gaps between the bands**.

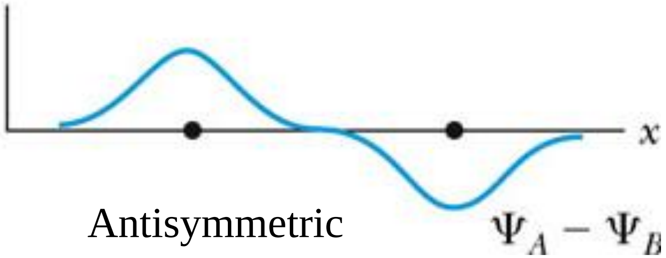
Consider initially the known wave functions of two atoms far enough apart so that they do not interact.



Interaction of the wave functions occurs as the atoms get closer



Symmetric



Antisymmetric

An atom in the symmetric state has a nonzero probability of being halfway between the two atoms, while an electron in the antisymmetric state has a zero probability of being at that location

- In the symmetric case the binding energy is slightly stronger resulting in a lower energy state.

Formation allowed and forbidden band
band theory of single-crystal materials.

For example silicon atoms contain fourteen atoms and configuration as $1s^2$ $2s^2$ $2p^6$ $3s^2$ $3p^2$ Ten of the fourteen silicon atom electrons occupy deep-lying energy levels (first and second state) and close and tightly bound to the nucleus .

The four remaining valence electrons are relatively weakly bound and are the electrons involved in chemical reactions. consider the n = 3 shell or level for the valence electrons.

The 3s $(3S^2)$state corresponds to n = 3 and I = 0 and contains two quantum states per atom. This state will contain two electrons at T = 0 K. The 3p state corresponds to n = 3 and I = 1 and contains six quantum states per atom. This state will contain the remaining two electrons $(3P^2)$ in the individual silicon atom. As the interatomic distance decreases or at equilibrium , the 3s and 3p states interact and overlap.

Hence discrete level split to the bands. Two allowed energy band and one forbidden band (energy gap)

1- four quantum state per atom are in the lower band called valance band (V_B) and allowed band may be filled from electron at absolute zero degree .

2- four quantum state per atom are in the upper band called conduction band and also allowed band but empty, at absolute zero degrees.

Energy gap (forbidden energy band): is energy gap between the top of the valance band to the bottom of the conduction band

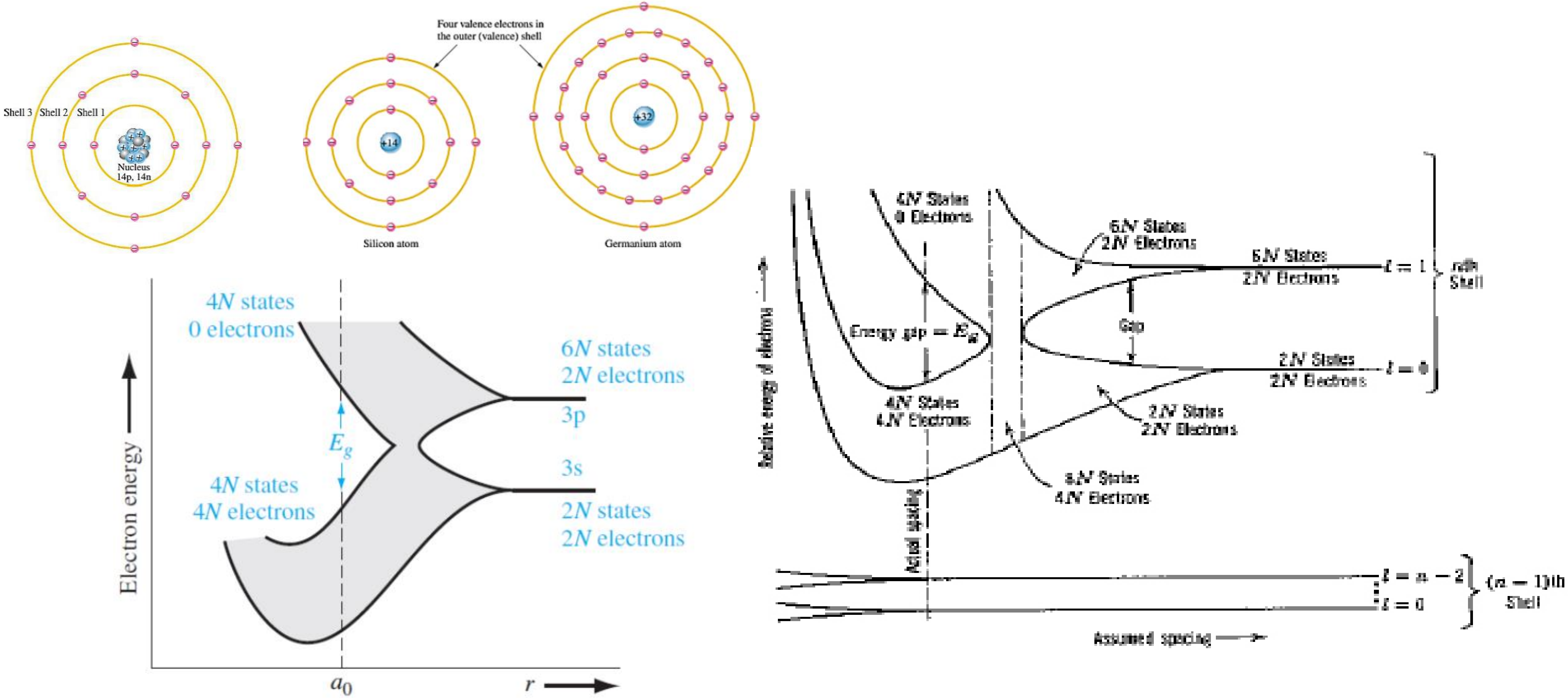


Figure 3.4 1 (a) Schematic of an isolated silicon atom. (h) The splitting of the 3s and 3p states **of** silicon into the allowed and forbidden energy bands

Band structure

Semiconductor - a solid in which the highest occupied energy band, the *valence band* (VB), is completely full at $T = 0°K$

However, the gap above this band is small, so that electrons may be excited thermally at room temperature from the valence band to the next-higher band

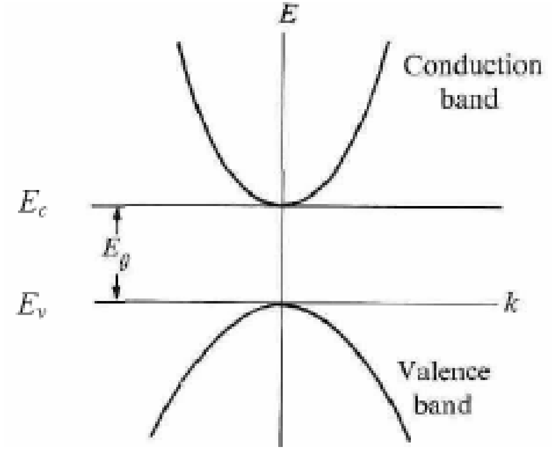
the conduction band (CB)

Electrons are excited across the gap → the bottom of the conduction band is populated by electrons, and the top of the valence band - by holes.

As a result, both bands are now only partially full → can carry a current if an electric field were applied

The energy of the CB has the form:

$$E_c(k) = E_c + \frac{\hbar^2 k^2}{2m_e}$$



The energy of the VB may be written as

$$E_v(k) = E_v - \frac{\hbar^2 k^2}{2m_h}$$

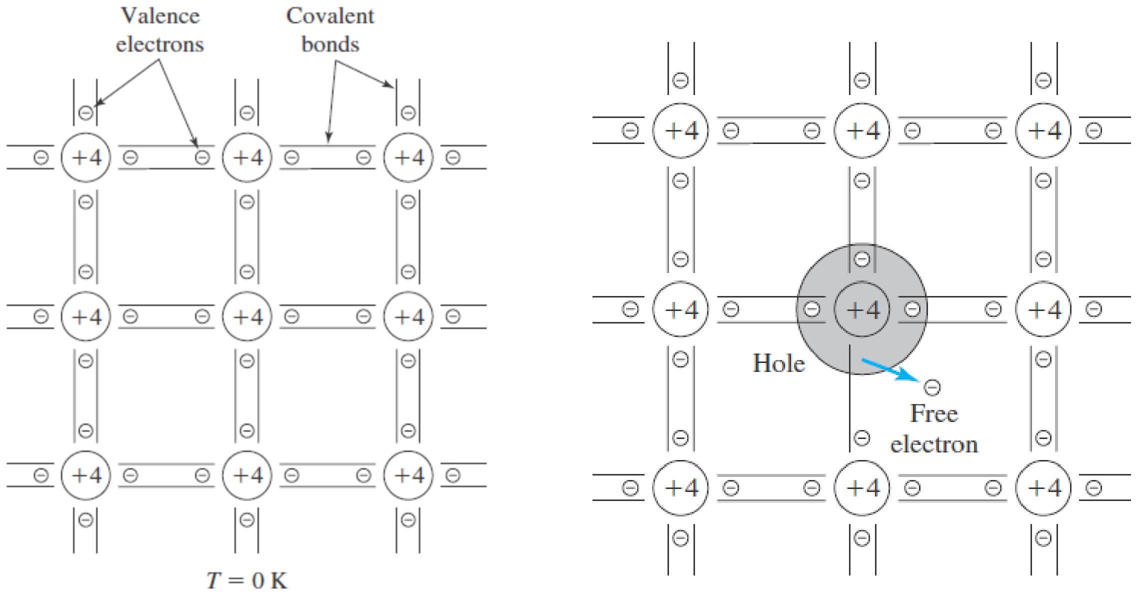
where k is wave number or the wave vector and m_n^* the effective mass of the electron. The energy E_g represents the energy gap. The zero-energy level is chosen to lie at the top of the VB.

Where m_h^* is the effective mass of the hole, that, because of the inverted shape of the VB, the mass of an electron at the top of the VB is negative, equal to $-m_h^*$ but the mass of a hole is positive.) only in the region c1ose to the top of the band, where most of the holes lie.

Two Types of Current Carrier in Semiconductors (generation of electron-hole pairs)

An important thing to note from Figure (a) below is that all the electrons are bound through covalent bonds only at the temperature of 0 K. There can be a certain number of brouken covalent bonds at temperatures higher than 0 K. This happens when the heat energy absorbed by a silicon atom is released through breakage of a covalent bond and release of a free electron that carries the energy away. The energy needed to break a covalent bond in silicon crystal is about 1.1 eV at room temperature, and it is slightly different at different temperatures. Obviously, there will be more broken covalent bonds at higher temperatures because the silicon atoms possess more thermal energy, which eventually destroys covalent bonds. When a silicon atom releases an electron, it becomes positively charged with a hole in its bond structure, as illustrated in Fig. (b)

The electrons released from covalent bonds broken by thermal energy (Fig.a) are mobile charged particles, so they can flow through the crystal to create electric current. Accordingly, we define the *free electrons* as current carriers.



$T = 0$ K

(a)

$T > 0$ K

(b)

Figure Two-dimensional representation of silicon crystal: (a) all the electrons are bound at 0 K, whereas at temperatures >0 K there are broken bonds, creating free electron–hole pairs (b).

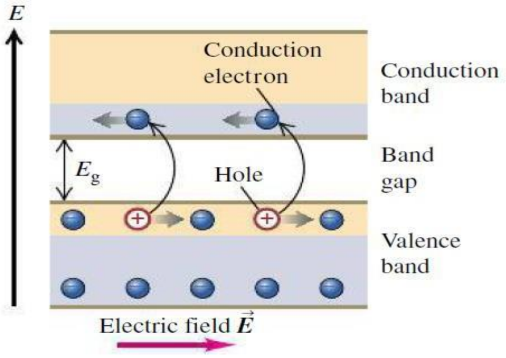


Fig: Current Carrier by electron and hole is applied electric fields in semiconductors

Semiconductor energy bands at room temperature (creating free electron–hole pairs)

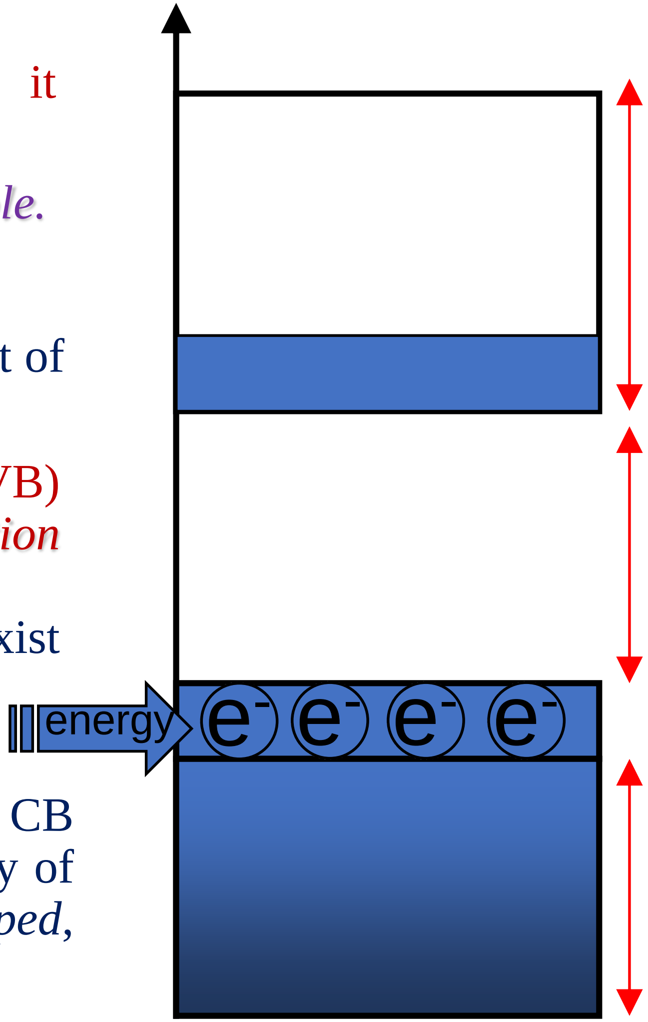
When enough *energy* is supplied to the e$^-$ sitting at the top of the valance band, e$^-$ can make a transition to the bottom of the conduction band

- When electron makes such a transition it leaves behind a *missing electron state.*
  - This missing electron state is called as a *hole*.
  - Hole behaves as a *positive charge carrier.*
- Magnitude of its charge is the same with that of the electron but with an opposite sign.

Holes contribute to current in *valance band* (VB) as e$^-$'s are able to create current in *conduction band* (CB).

Hole is *not* a free particle. It can only exist within the crystal. A hole is simply

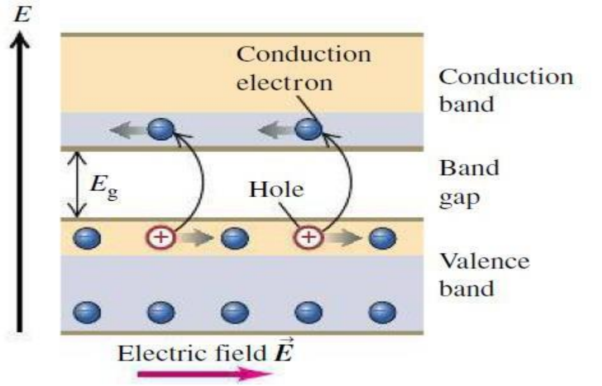
A transition results an equal number of e$^-$ in CB and holes in VB. This is an important property of *intrinsic*, or *undoped s/c's*. For *extrinsic*, or *doped*, semiconductors this is no longer true.



Empty conduction band

Forbidden energy gap [Eg]

Full valance band



Figu: whereas at temperatures >0 K creating free electron–hole pairs.

Temperature dependence of the energy bandgap

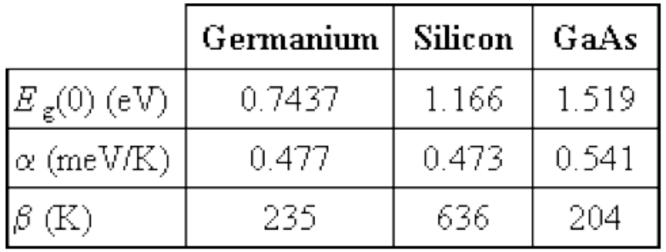
The energy bandgap of semiconductors tends to decrease as the temperature is increased. Which that the interatomic spacing increases when the amplitude of the atomic vibrations increases due to the increased thermal energy.

This effect is quantified by the linear expansion coefficient of a material. An increased interatomic spacing decreases the average potential seen by the electrons in the material, which in turn reduces the size of the energy bandgap.

The temperature dependence of the energy bandgap, *E*g, has been experimentally determined yielding the following expression for *E*g as a function of the temperature, *T*:

$$E_g(T) = E_g(0) - \frac{\alpha T^2}{T + \beta}$$

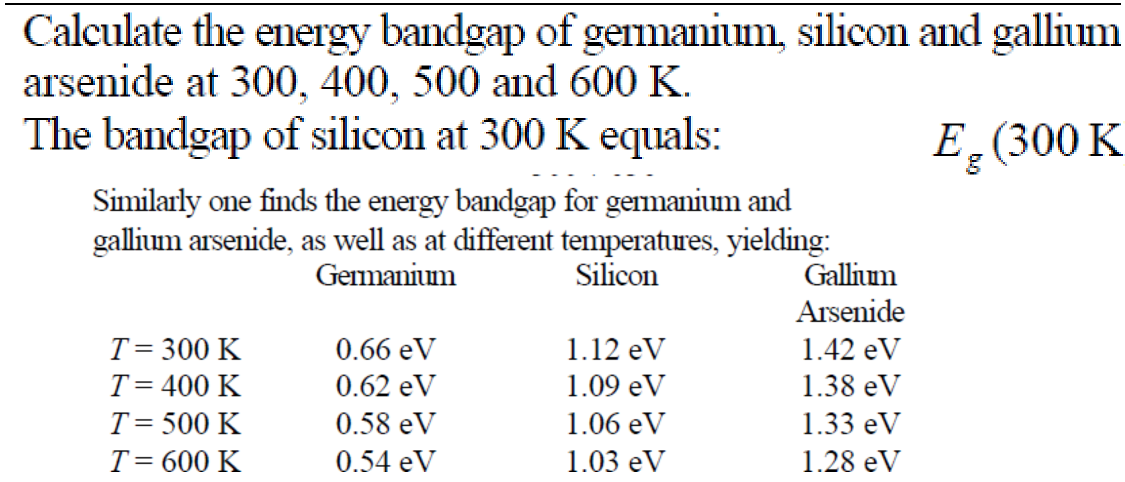
where *E*g(0), *α* and *β* are the fitting parameters. These fitting parameters are listed for germanium, silicon and gallium arsenide in Table



	Germanium	Silicon	GaAs
$E_g(0)$ (eV)	0.7437	1.166	1.519
α (meV/K)	0.477	0.473	0.541
β (K)	235	636	204

Parameters used to calculate the energy bandgap of germanium, silicon and gallium arsenide (GaAs) as a function of temperature

A plot of the resulting bandgap versus temperature is shown in Figure below for germanium, silicon and gallium arsenide



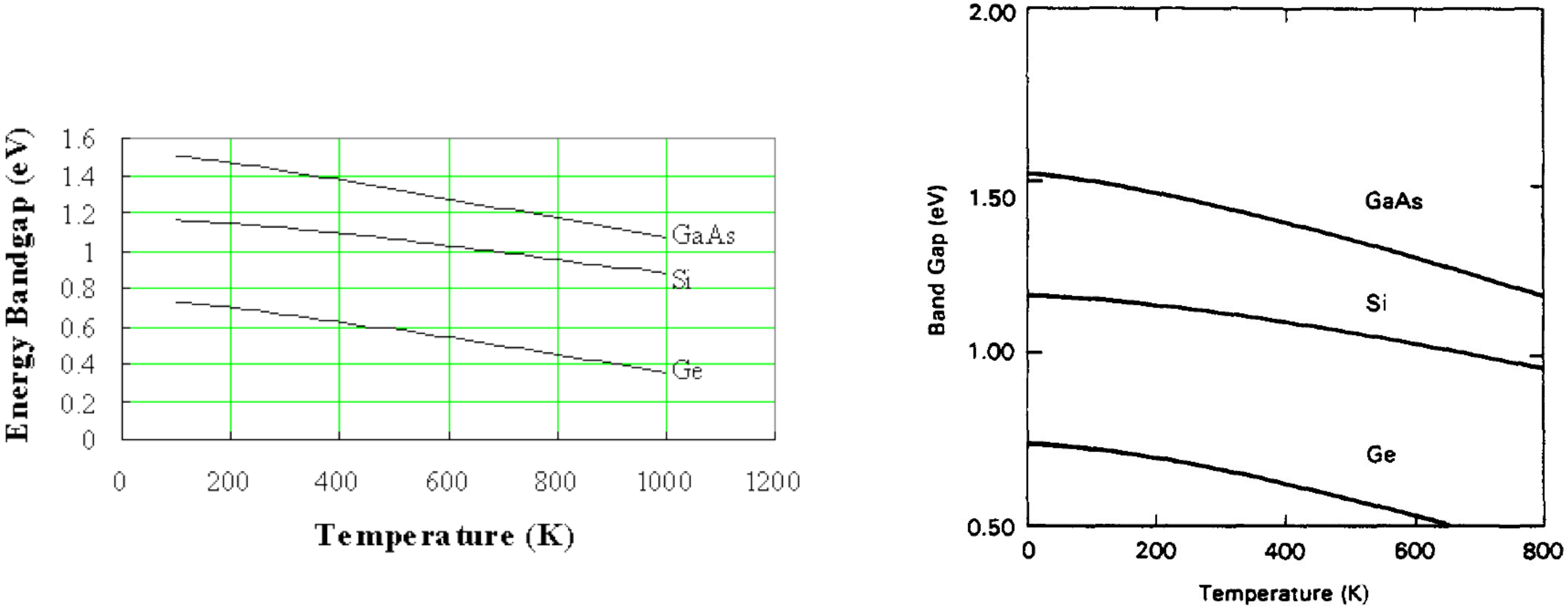
Calculate the energy bandgap of germanium, silicon and gallium arsenide at 300, 400, 500 and 600 K.

The bandgap of silicon at 300 K equals:

$$E_g(300\,\mathrm{K}) = E_g(0\,\mathrm{K}) - \frac{\alpha T^2}{T + \beta} = 1.166 - \frac{0.473 \times 10^{-3} \times (300)^2}{300 + 636} = 1.12\ \mathrm{eV}$$

Similarly one finds the energy bandgap for germanium and gallium arsenide, as well as at different temperatures, yielding:

	Germanium	Silicon	Gallium Arsenide
T = 300 K	0.66 eV	1.12 eV	1.42 eV
T = 400 K	0.62 eV	1.09 eV	1.38 eV
T = 500 K	0.58 eV	1.06 eV	1.33 eV
T = 600 K	0.54 eV	1.03 eV	1.28 eV



Temperature dependence of the energy bandgap of germanium (Ge), silicon (Si) and gallium arsenide (GaAs).

Example: Calculate the energy bandgap of germanium, silicon and gallium arsenide at 300, 400, 500 and 600 K.

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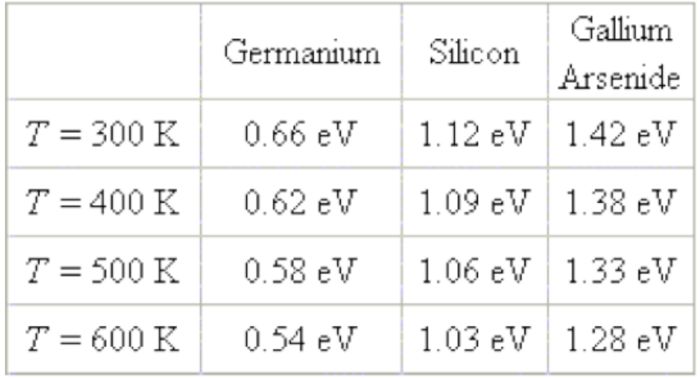

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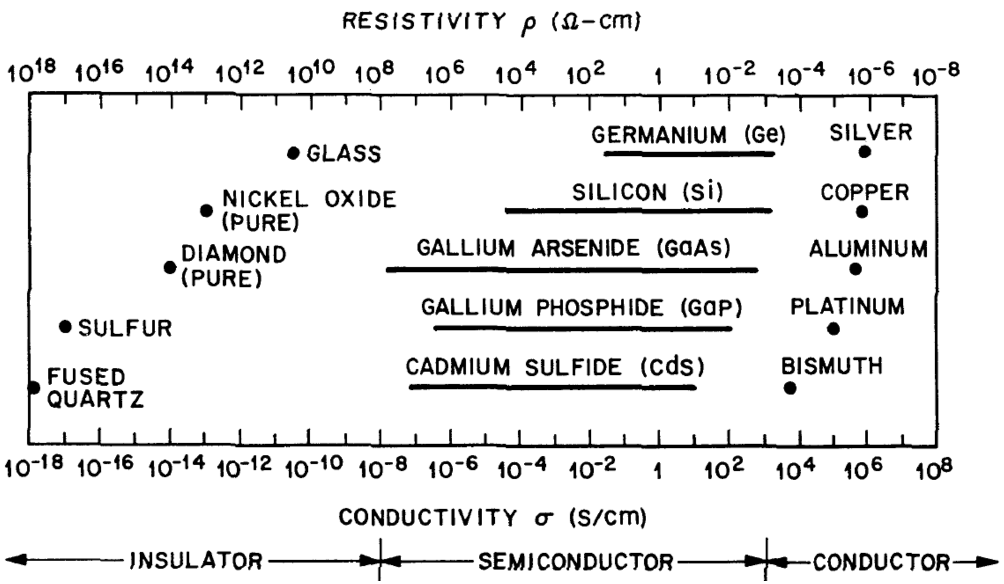
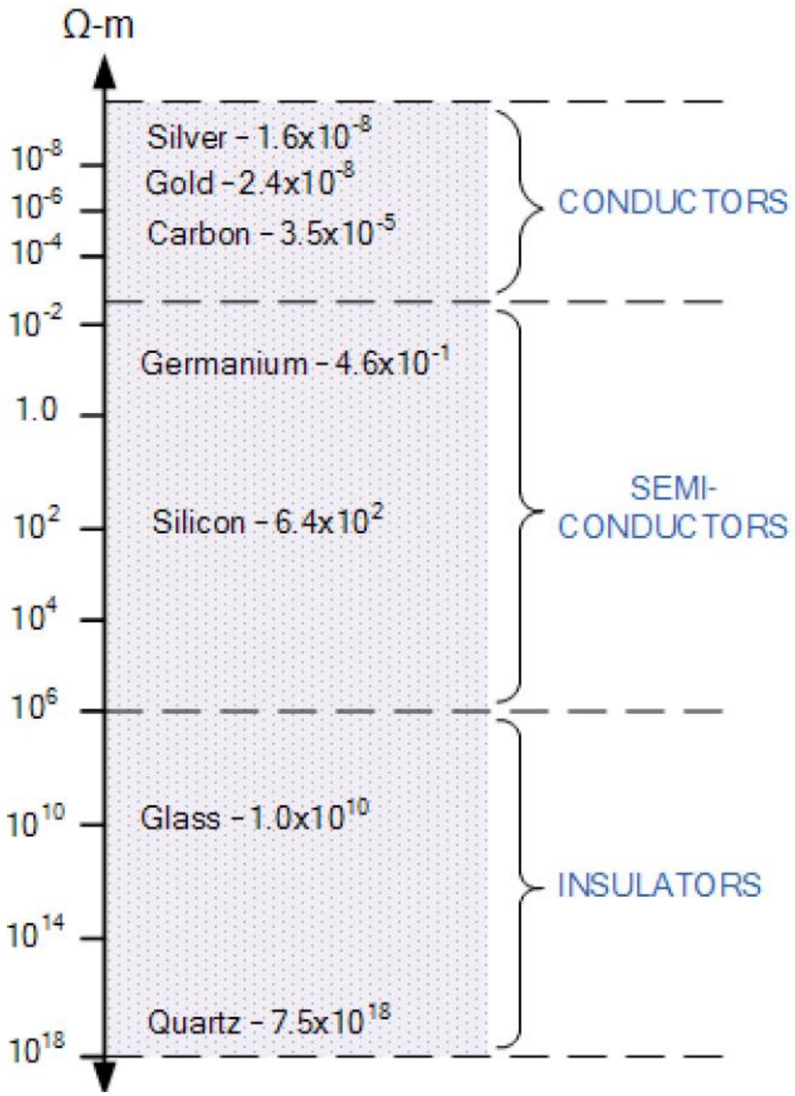
- **Band Theory of Solids**
- **Semiconductor Theory**
- **There are three categories of solids, based on their conducting properties:**
  - **conductors semiconductor insulators**

This table reveals that

- **The electrical conductivity at room temperature is quite different for each of these three kinds of solids**
  - **Metals and alloys have the highest conductivities**
  - **followed by semiconductors and then by insulators**

the resistivity of semiconductors, ρ, is typically between 10^{-2} and 10^{8} Ω-cm. And conductivity (σ) 10^{8} to 10^{-2} $\frac{s}{cm}$





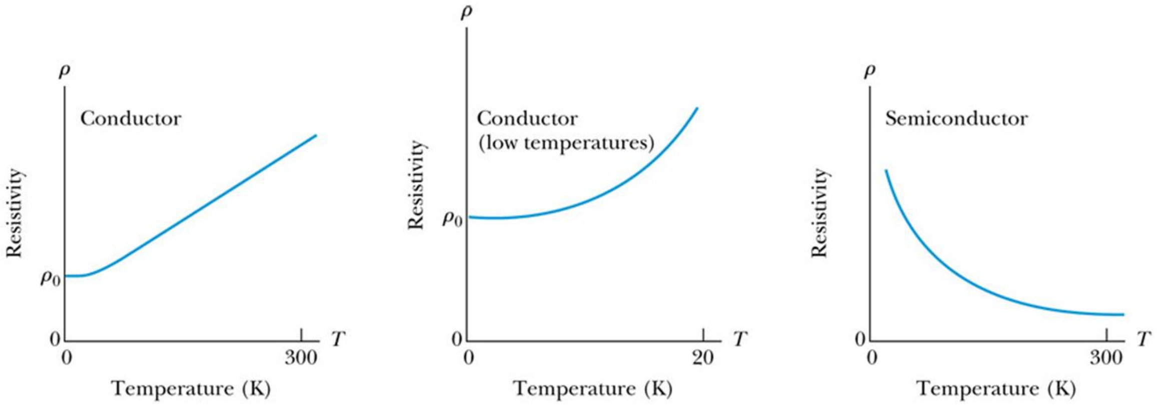
Typical range of conductivities for insulators, semiconductors, and conductors.

Semiconductor Conduction

- The **free-electron** model does not apply to semiconductors and insulators, since these materials simply lack enough free electrons to conduct in a free-electron mode.

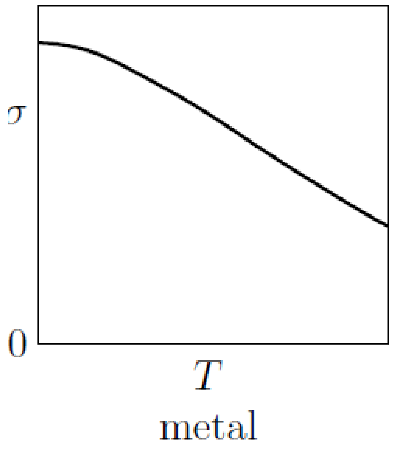
  There is a different conduction mechanism for semiconductors than for normal conductors.

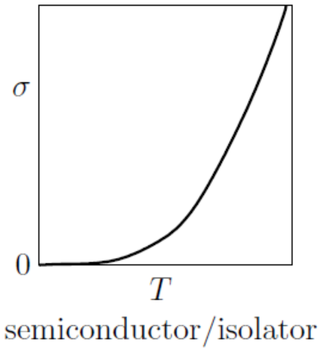
Resistivity vs. Temperature



(a) (b) (c)

Figure : (a) Resistivity versus temperature for a typical conductor. Notice the linear rise in resistivity with increasing temperature at all but very low temperatures. (b) Resistivity versus temperature for a typical conductor at very low temperatures. Notice that the curve flattens and approaches a nonzero resistance as $T \rightarrow 0$. (c) Resistivity versus temperature for a typical semiconductor. The resistivity increases dramatically as $T \rightarrow 0$.





Schematic temperature dependence of the electric conductivity for semiconductors

The properties of semiconductor

- 1- Valence band is the highest range of electron energies in which electrons are normally present at absolute zero temperature.
- 2- In order for an electron to jump from a valence band to a conduction band, it requires a specific amount of energy for the transition.

- 3-The required energy differs with different materials.
- 4-The conductivity of intrinsic semiconductors is strongly dependent on the band gap.

5-The resistivity of semiconductor is in order of 1 ev.

6-The band gap energy F_g, of an semiconductor is usually on the Order is of 1 ev or larger, so that at room temperature, there are essentially no electrons in the conduction band and the valence band remains completely full.

The number of hole in the valance band equal the number of electron conduction band

7 - resistivity decrease with increasing temperature and conductivity increase

8- semiconductor is a material that is between conductors and insulators in its ability to conduct electrical current.

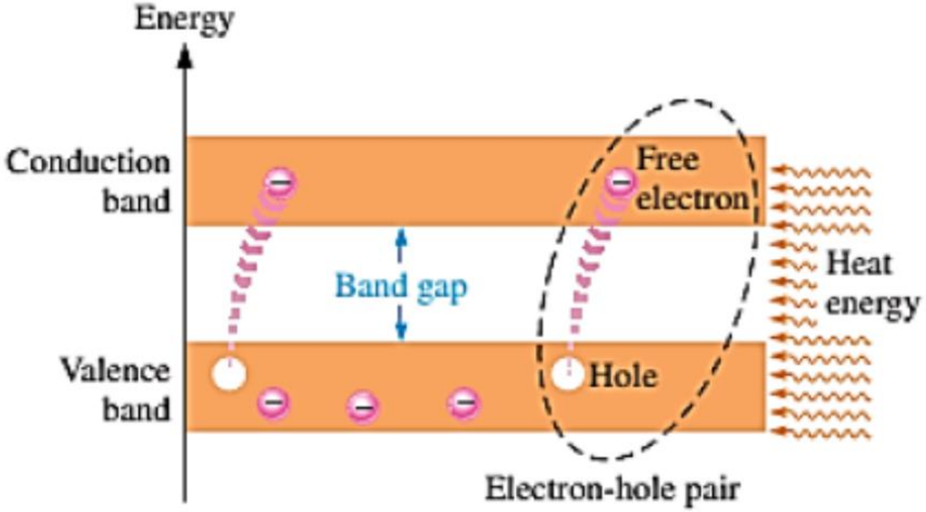


Figure energy bands of semiconductor: upper band is conduction band and lower band is valence band both are allowed bands, but energy gap is forbidden band

At $Temperature > 0\,K$ Creation of electron−hole pairs in semiconductror crystal

Insulators

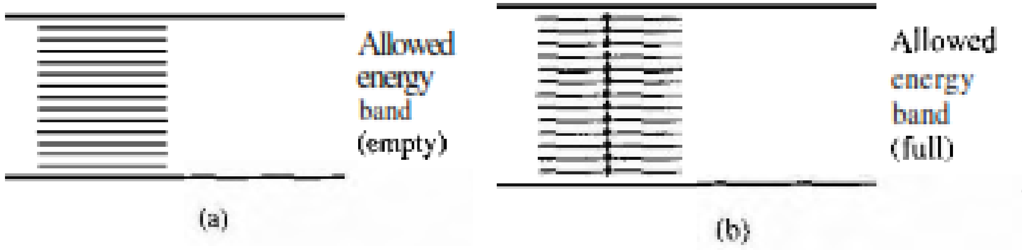
There are two an allowed energy band, valance band that is completely filled of electrons and conduction band empty from electron.

If an electric field is applied to upper band (conduction band), empty from electrons, there are no particles to move, so there will be no current

Shows another allowed energy band, lower band (valance band) whose energy states are completely filled of electrons.

that a completely fill energy band will also not give rise to a current because there is charge cannot moving A material that has energy is an insulator bands either completely empty or completely full as shown in below figure

An insulator is a material that does not conduct electrical current under normal conditions. Valence electrons are tightly bound to the atoms; therefore, there are very few free electrons in an insulator. Energy gap in an insulator is very wide (≥6eV). Valence electron requires a large electric field to gain enough energy to jump into conduction band. Examples of insulators are rubber, plastics, glass, mica, and quartz.



Allowed energy band empty

Allowed energy band full

Figure: allowed energy band showing a- an empty band - a completely full band

The properties of insulator

1-The resistivity of an insulator is very large.

2- the conductivity of an insulator is very small.

3-There are essentially no charged particle that can contribute to a drift current

4-The band gap energy Type equation here. **E_g, of an insulator is usually on the Order of 3.5 to 6 eV or larger, so that at room temperature, there are essentially no electrons in the conduction band and the valence band remains completely full.**

conductor

Conduction band CB parity filled from electron at ordinary temperature and valance band VB completely filled at only at absolute zero temperature as shown in fig

The conduction band and the valance band overlap at equilibrium distance

characteristic of metal or conductors

1-very low value of resistivity

2-many electron a valible of conduction current

3-exhabit very large electrical conductivity

4-there are no band gap

5- resistivity increase with increasing temperature but conductivity decrease

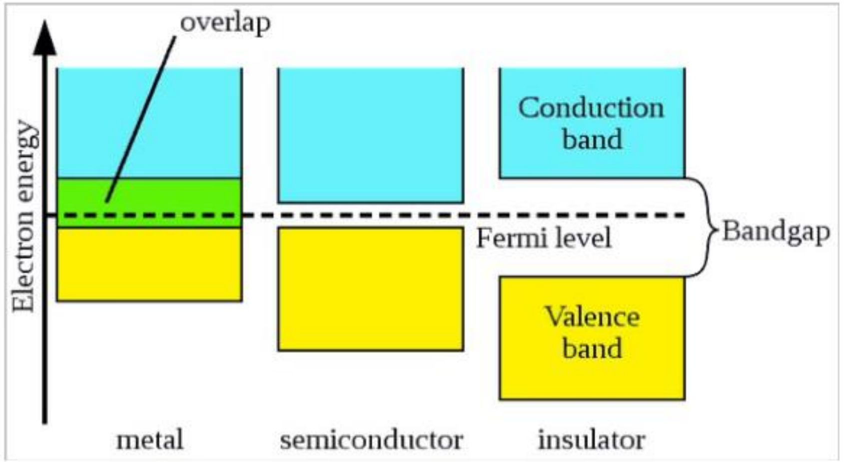


Figure Two possible energy bands of a metal showing (a) a partially filled band and (b) overlapping allowed energy bands.