ENERGY BANDS IN SOLIDS

Energy Bands

When a number of atoms are brought close together to form a crystal, each atom will exert an electric force on its neighbors. As a result of this interatomic coupling, the crystal forms a single electronic system obeying Pauli's exclusion principle. Therefore, each energy level of the isolated atom splits into as many energy levels as there are atoms in the crystal, so that Pauli's exclusion principle is satisfied. The separation between the split-off energy levels is very small. This large number of discrete and closely spaced energy levels form an ***energy band***. Energy bands are represented schematically by shaded regions in Fig.1.2

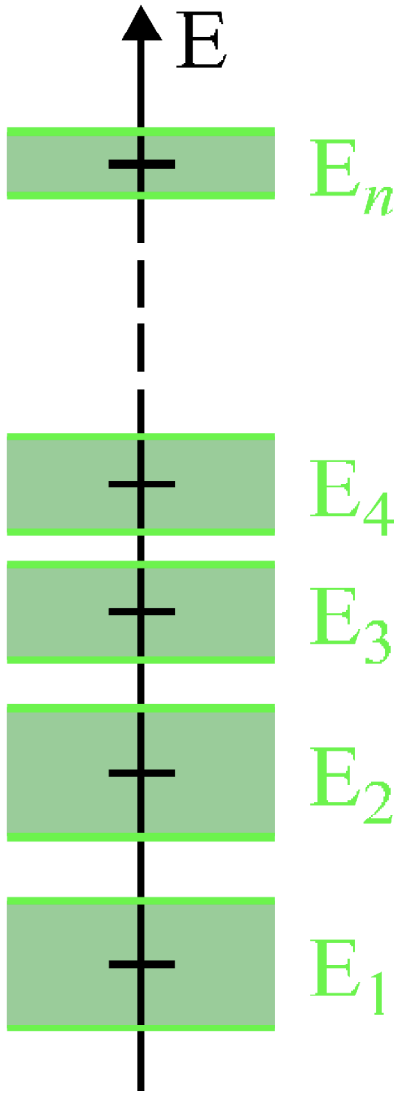


Fig 1.1. Discrete energy levels

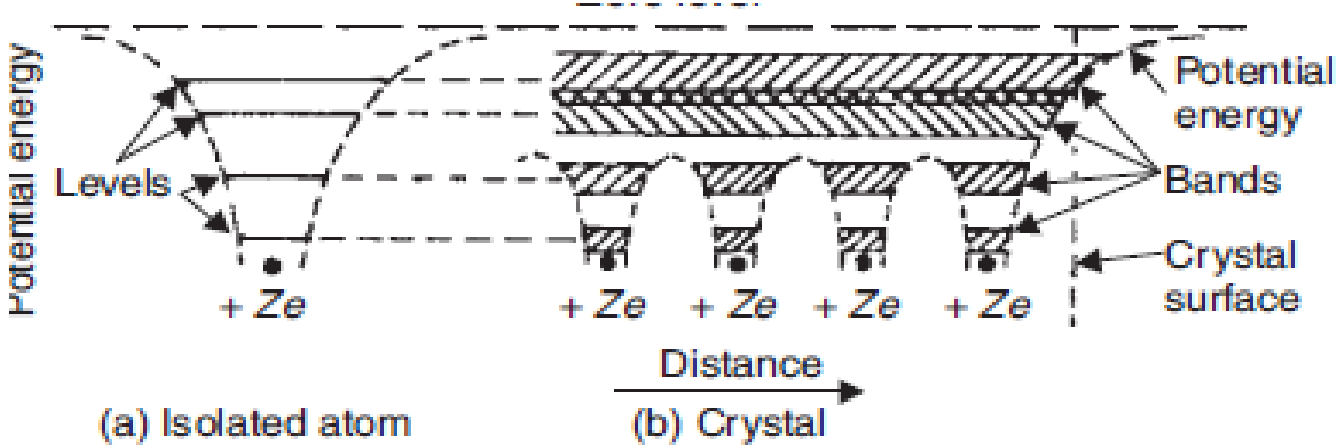


Fig. 1.2 Splitting of energy levels of isolated atoms into energy bands as these atoms are brought close together to produce a crystal.

The width of a band is independent of the number of atoms in the crystal, but the number of energy levels in a band is equal to the number of atoms in the solid. Consequently, **as the number of atoms in the crystal increases, the separation between the energy levels in a band decreases**. As the crystal contains a large number of atoms ($\approx 10^{29}$ m–3), the spacing between the discrete levels in a band is so small that the band can be treated as continuous.

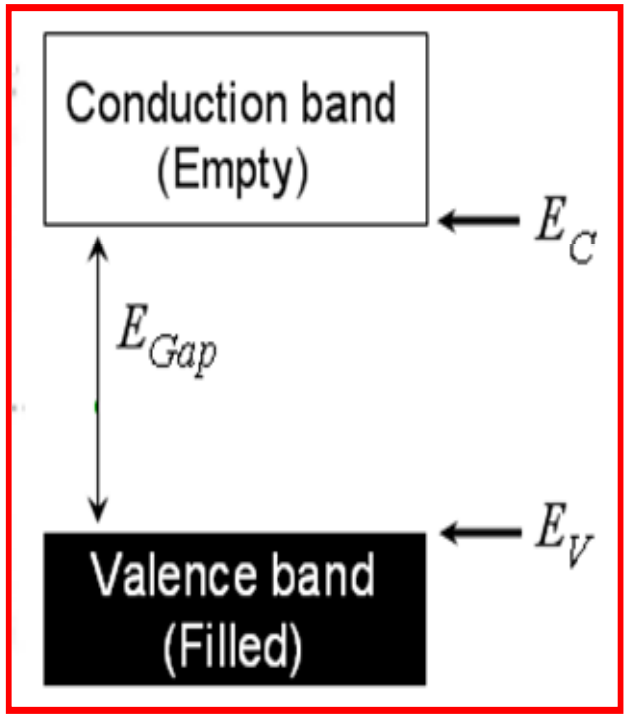
The **lower energy bands are normally completely filled** by the electrons since the electrons always tend to occupy the lowest available energy states. The **higher energy bands may be completely empty or may be partly filled** by the electrons. Pauli's exclusion principle restricts the number of electrons that a band can accommodate. A partly filled band appears when a partly filled energy level produces an energy band or when a totally filled band and a totally empty band overlap.

As the allowed energy levels of a single atom expand into energy bands in a crystal, the electrons in a crystal cannot have energies in the region between two successive bands. In other words, the energy bands are separated by gaps of ***forbidden energy***.

1. The last completely filled (at leastat T = 0 K) band is called the Valence Band

2. The next band with higher energy is the **Conduction Band** The Conduction Band can be empty or partially filed

3. The energy difference between the bottom of the CB and the top of the VB is called the **Band Gap** (or **Forbidden Gap**)



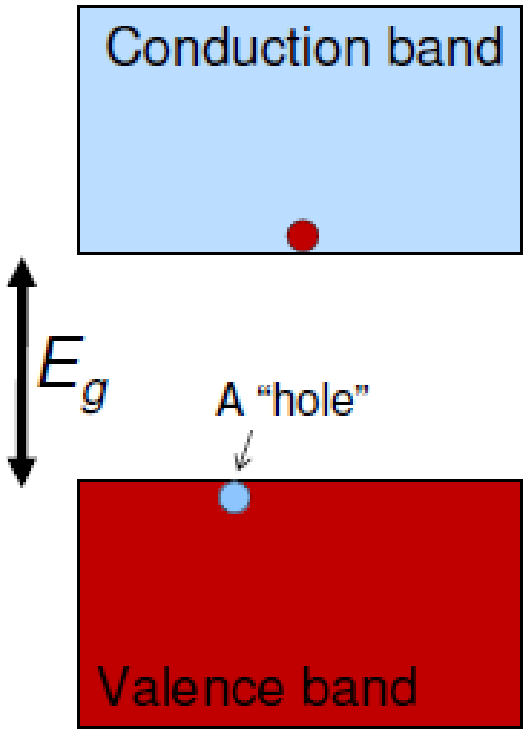
Thermal excitation of electrons

• The removal of an electron from the valence band leaves behind a gap in the electrons forming the bonds

• These act like positively charged carriers,

zand are called *holes*

• You can view their behavior as resembling bubbles moving in a liquid



On the basis of the band structure, crystals can be classified into metals, insulators, and semiconductors

Metal

A solid which contains a partly filled band structure is called a *metal. Under the influence of an applied electric field the electrons may acquire* additional energy and move into higher states. Since these mobile electrons constitute a current, this substance is a good conductor of electricity and the partly filled region is the conduction band. *The electrons in the conduction band are known as free electrons or conduction electrons.* One example of the band structure of a metal is given in Fig. 1-3a, which shows overlapping valence and conduction bands.

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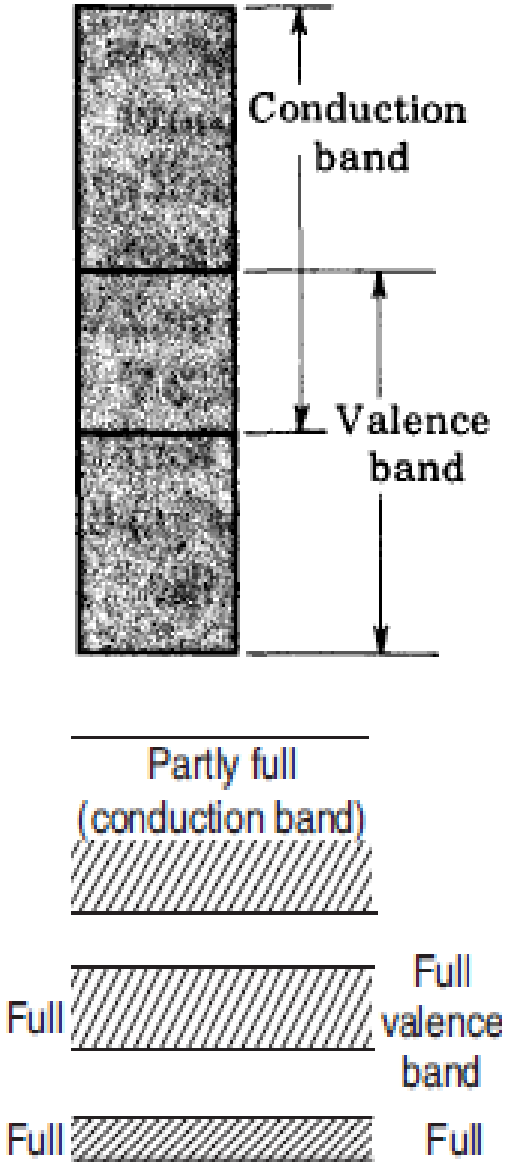
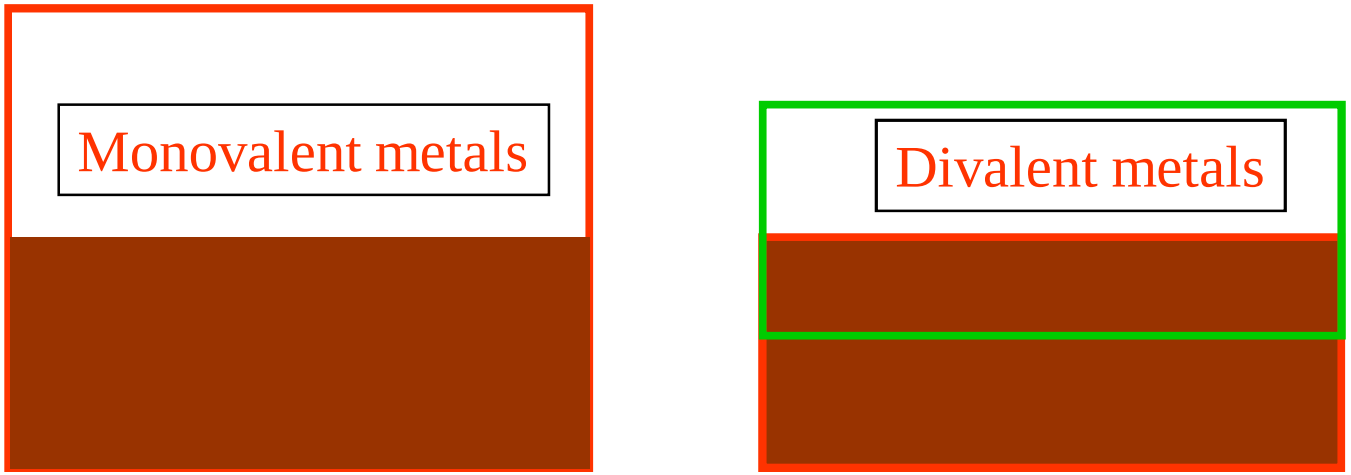


Fig. **1-3a,**

Energy band diagram: METALS



- Monovalent metals: Ag, Cu, Au → 1 e^- in the outermost orbital
  ⇒ outermost energy band is only half filled
- Divalent metals: Mg, Be → overlapping conduction and valence bands
  ⇒ they conduct even if the valence band is full
- Trivalent metals: Al → similar to monovalent metals!!!
  ⇒ outermost energy band is only half filled !!!

Insulator

In some crystalline solids, the forbidden energy gap between the uppermost filled band, calledthe *valence band, and the lowermost empty band, called the conduction band, is very large. In* such solids, at ordinary temperatures only a few electrons can acquire enough thermal energy to move from the valence band into the conduction band. Such solids are known as *insulators.* Since only a few free electrons are available in the conduction band, an insulator is a bad conductor of electricity. Diamond having a forbidden gap of 6 eV is a good example of an insulator. The energy band structure of an insulator is schematically shown in Fig. 1.3(*b).*

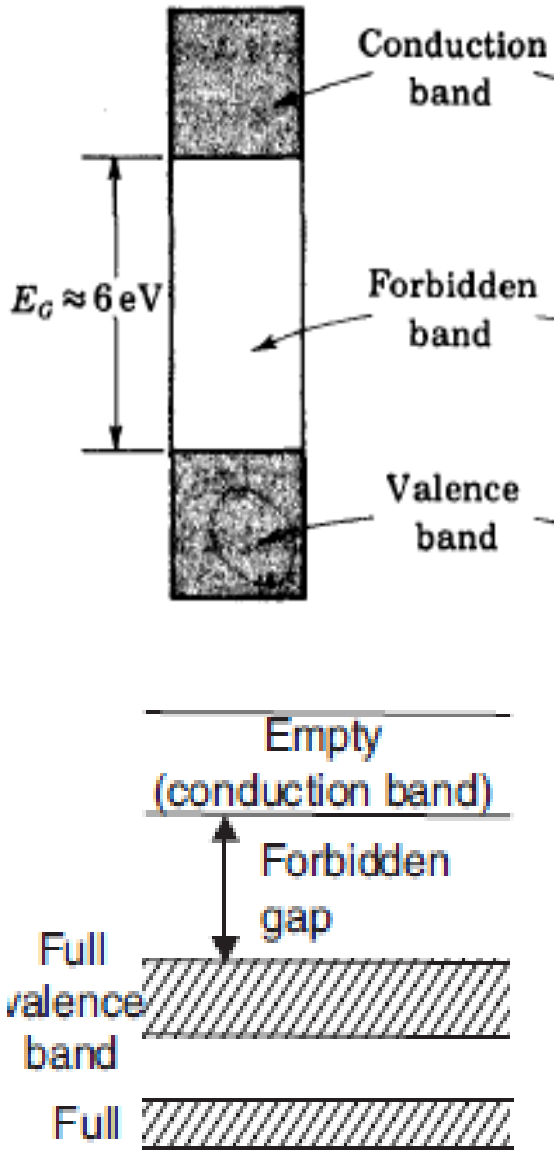
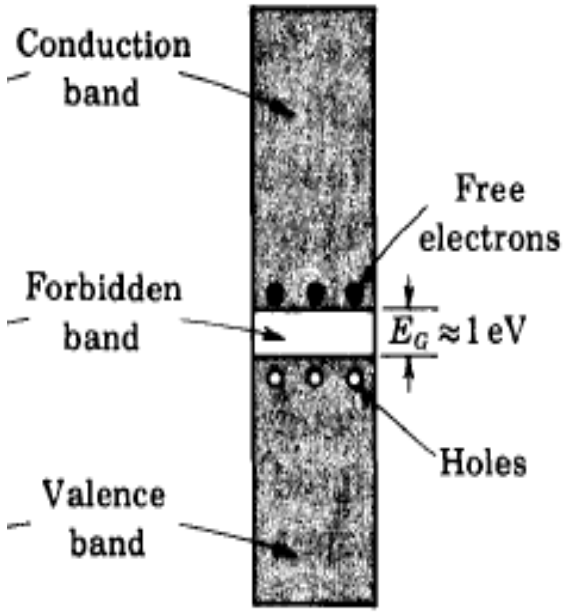
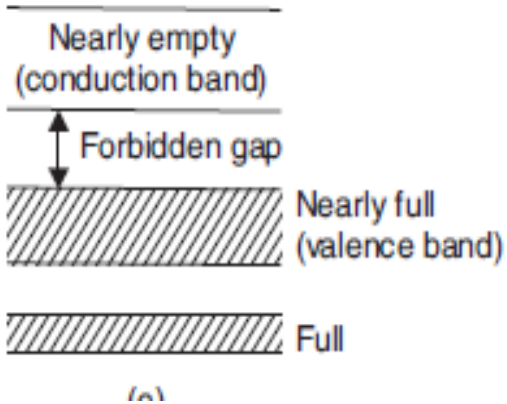


Fig. 1-3b

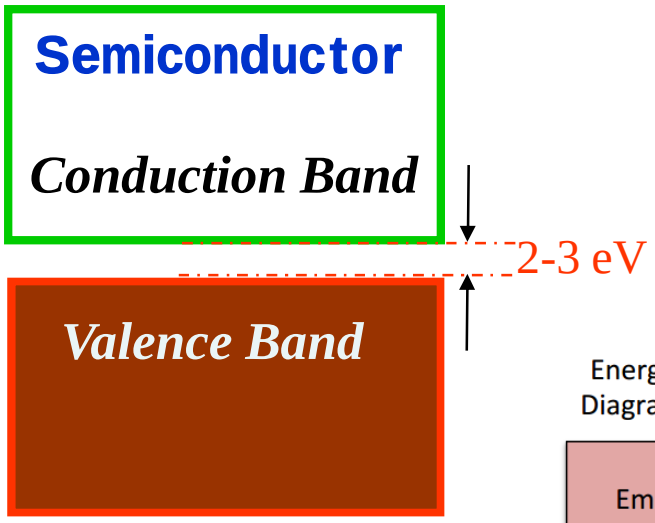
Semiconductor

A substance for which the width of the forbidden energy region is relatively small (-1 eV) is called a semiconductor. Graphite, a crystalline form of carbon but having a crystal symmetry which is different from diamond, has such a small value of E G , and it is a semiconductor. The most important practical semiconductor materials are germanium and silicon, which have values of EG of 0.785 and 1.21 eV, respectively, at O°K. Energies of this magnitude normally cannot be acquired from an applied field. Hence the valence band remains full, the conduction band empty, and these materials are insulators at low temperatures. However, the conductivity increases temperature, as we explain below. These substances are known as intrinsic (pure) semiconductors.

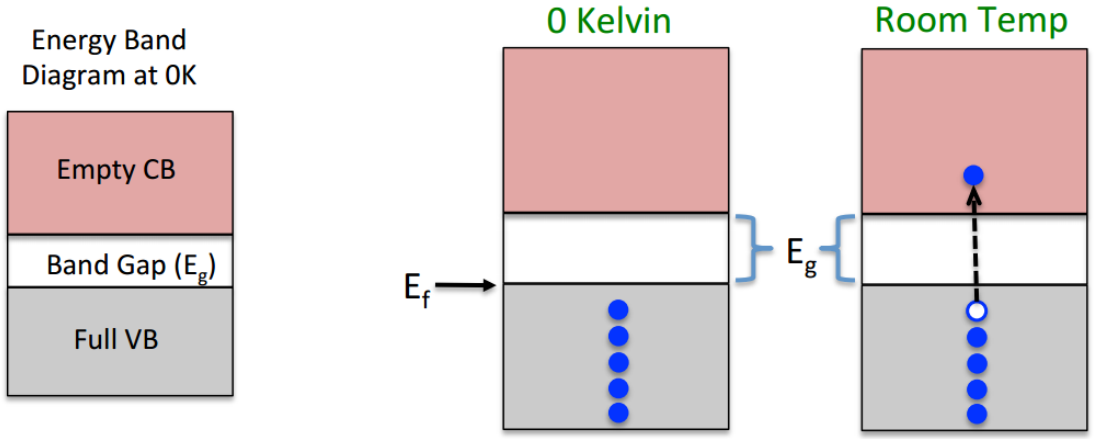




Energy band diagram: SEMICONDUCTORS



Band Gaps of some intrinsic semiconductors							
Material	Si	Ge	GaP	GaAs	InSb	CdS	ZnTe
Band Gap (eV)	1.11	0.67	2.25	1.42	0.17	2.4	2.26



- Elements of the 4th column (C, Si, Ge, Sn, Pb) → valence band full but no overlap of valence and conduction bands
- Diamond → PE as strong function of the position in the crystal
  ⇨ Band gap is 5.4 eV
- Down the 4th column the outermost orbital is farther away from the nucleus and less bound ⇒ the electron is less strong a function of the position in the crystal ▶ reducing band gap down the column

Since the band-gap energy of a crystal is s function of interatomic spacing **it is not surprising that EG depends somewhat on temperature.** I t has been determined experimentally that EG decreases with temperature,

Energy gaps (room temperature)

Material	E_g (eV)	Observed electrical behaviour
SiO_2	9.0	Insulator
Diamond	5.5	Insulator
GaAs	1.42	Semiconductor
Silicon	1.12	Semiconductor
Germanium	0.66	Semiconductor
Cu	0	Metal
Ag	0	Metal
Au	0	Metal