Semiconductor: Types and Band structure

What are Semiconductors?

Semiconductors are the materials which have a **conductivity and resistivity in between conductors** (generally metals) and non-conductors or **insulators** (such ceramics). Semiconductors can be compounds such as gallium arsenide or pure elements, such as germanium or silicon.

Properties of Semiconductors

Semiconductors can conduct electricity under preferable conditions or circumstances. This unique property makes it an excellent material to conduct electricity in a controlled manner as required.

Unlike conductors, the charge carriers in semiconductors arise only because of external energy (thermal agitation). It causes a certain number of valence electrons to cross the energy gap and jump into the conduction band, leaving an equal amount of unoccupied energy states, i.e. holes. Conduction due to electrons and holes are equally important.

- **Resistivity:** 10^{-5} to 10^{6} Ωm
- **Conductivity:** 10^{5} to 10^{-6} mho/m
- **Temperature coefficient of resistance:** Negative
- **Current Flow:** Due to electrons and holes
- Semiconductor acts like an insulator at Zero Kelvin. On increasing the temperature, it works as a conductor.
- Due to their exceptional electrical properties, semiconductors can be modified by doping to make semiconductor devices suitable for energy conversion, switches, and amplifiers.
- Lesser power losses.
- Semiconductors are smaller in size and possess less weight.
- Their resistivity is higher than conductors but lesser than insulators.
- The resistance of semiconductor materials decreases with the increase in temperature and vice-versa.

Examples of Semiconductors:

Gallium arsenide, germanium, and silicon are some of the most **commonly used semiconductors**. Silicon is used in electronic circuit fabrication and gallium arsenide is used in solar cells, laser diodes, etc.

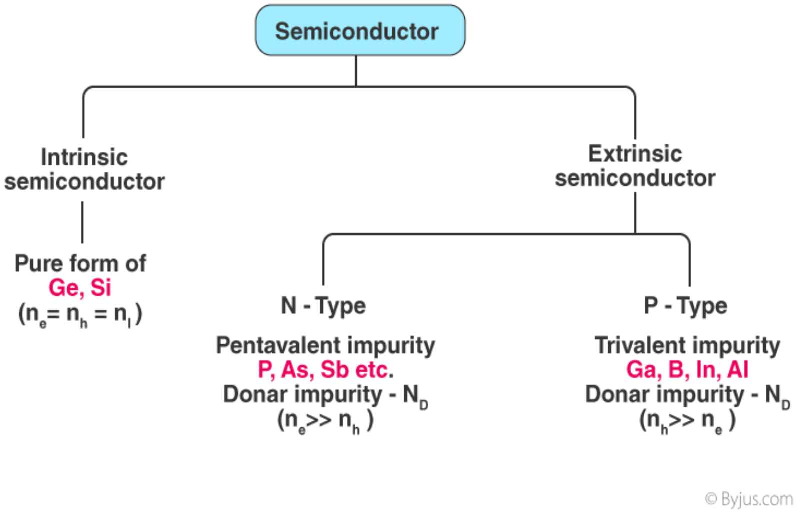
Types of Semiconductors

Semiconductors can be classified as:

- **Intrinsic Semiconductor**
- **Extrinsic Semiconductor**

Intrinsic Semiconductor

An **intrinsic type of semiconductor material** is made to be very pure chemically. It is made up of only a single type of element. Germanium (Ge) and Silicon (Si) are the most common type of intrinsic semiconductor elements. They have four valence electrons (tetravalent). They are bound to the atom by



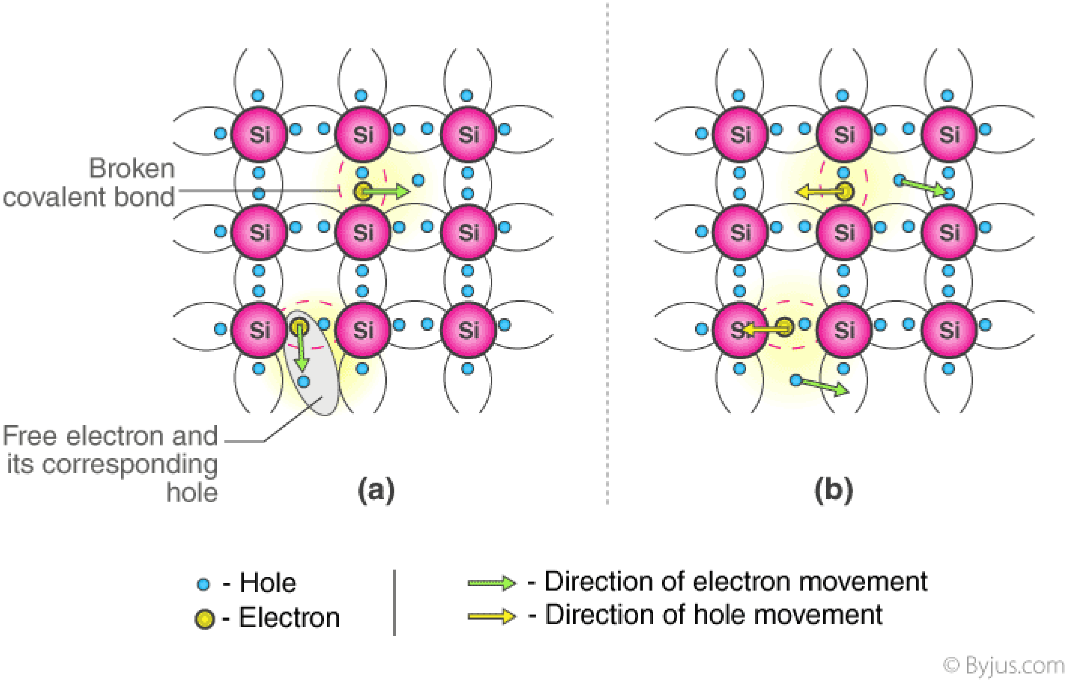
covalent bond at absolute zero temperature.

When the temperature rises, due to collisions, few electrons are unbounded and become free to move through the lattice, thus creating an absence in its original position (hole). These free electrons and holes contribute to the conduction of electricity in the semiconductor. The negative and positive charge carriers are equal in number.

The thermal energy is capable of ionizing a few atoms in the lattice, and hence their conductivity is less.

Lattice of Pure Silicon Semiconductor at Different Temperatures

- **At absolute zero kelvin temperature:** At this temperature, the covalent bonds are very strong and there are no free electrons and the semiconductor behaves as a perfect insulator.
- **Above absolute temperature:** With the increase in temperature few valence electrons jump into the conduction band and hence it behaves like a poor conductor.

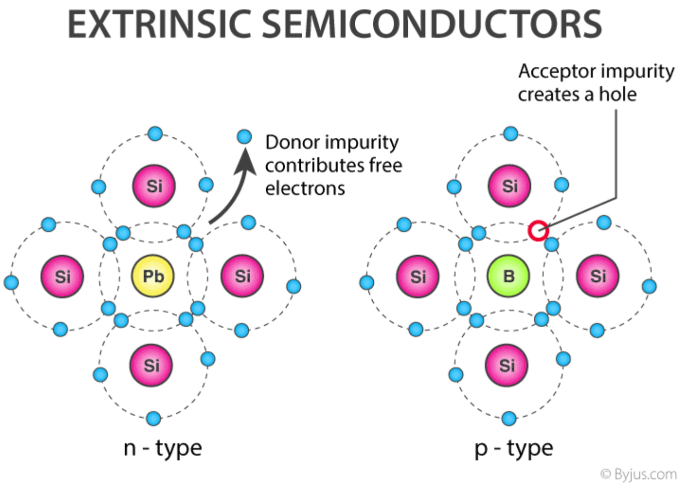


Conduction Mechanism in Case of Intrinsic Semiconductors (a) In absence of electric field (b) In presence of electric Field

Extrinsic Semiconductor

The conductivity of semiconductors can be greatly improved by introducing a small number of suitable replacement atoms called IMPURITIES. The process of adding impurity atoms to the pure semiconductor is called DOPING. Usually, only 1 atom in 10^7 is replaced by a dopant atom in the doped semiconductor. An extrinsic semiconductor can be further classified into:

- **N-type Semiconductor**
- **P-type Semiconductor**



Classification of Extrinsic Semiconductor

N-Type Semiconductor

- Mainly due to electrons
- Entirely neutral
- $I = I_h$ and $n_h >> n_e$
- Majority – Electrons and Minority – Holes

When a pure semiconductor (Silicon or Germanium) is doped by pentavalent impurity (P, As, Sb, Bi) then, four electrons out of five valence electrons bonds with the four electrons of Ge or Si.

The fifth electron of the dopant is set free. Thus the impurity atom donates a free electron for conduction in the lattice and is called "**Donar**".

Since the number of free electron increases by the addition of an impurity, the negative charge carriers increase. Hence it is called n-type semiconductor.

Crystal as a whole is neutral, but the donor atom becomes an immobile positive ion. As conduction is due to a large number of free electrons, the electrons in the n-type semiconductor are the MAJORITY CARRIERS and holes are the MINORITY CARRIERS.

P-Type Semiconductor

- Mainly due to holes
- Entirely neutral
- $I = I_h$ and $n_h >> n_e$
- Majority – Holes and Minority – Electrons

When a pure semiconductor is doped with a trivalent impurity (B, Al, In, Ga) then, the three valence electrons of the impurity bonds with three of the four valence electrons of the semiconductor.

This leaves an absence of electron (hole) in the impurity. These impurity atoms which are ready to accept bonded electrons are called "**Acceptors**".

With the increase in the number of impurities, holes (the positive charge carriers) are increased. Hence, it is called p-type semiconductor.

Crystal as a whole is neutral, but the acceptors become an immobile negative ion. As conduction is due to a large number of holes, the holes in the p-type semiconductor are MAJORITY CARRIERS and electrons are MINORITY CARRIERS.

Difference between Intrinsic and Extrinsic Semiconductors

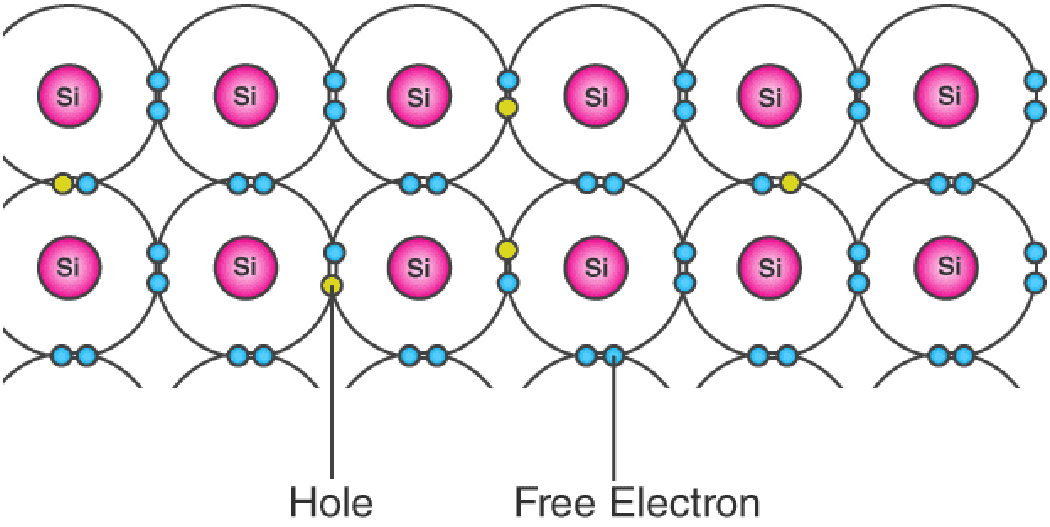
Intrinsic Semiconductor	**Extrinsic Semiconductor**
Pure semiconductor	Impure semiconductor
Density of electrons is equal to the density of holes	Density of electrons is not equal to the density of holes
Electrical conductivity is low	Electrical conductivity is high
Dependence on temperature only	Dependence on temperature as well as on the amount of impurity

No impurities	Trivalent impurity, pentavalent impurity

Holes and Electrons in Semiconductors

Holes and electrons are the types of charge carriers accountable for the flow of current in semiconductors. **Holes** (valence electrons) are the positively charged electric charge carrier whereas **electrons** are the negatively charged particles. Both electrons and holes are equal in magnitude but opposite in polarity.

The **bond model** of electrons in silicon of valency 4 is shown below. Here, when one of the free electrons (blue dots) leaves the lattice position, it creates a hole (grey dots). This hole thus created takes the opposite charge of the electron and can be imagined as positive charge carriers moving in the lattice.



Concept of Electrons and Holes in Semiconductors

Band Formation in crystals

We know that the electrons in an atom are present in different energy level. When we try to assemble a lattice of a solid with N atoms, then each level of an atom must split up into N levels in the solid. This splitting up of sharp and tightly packed energy levels forms **Energy Bands**. The gap between adjacent bands representing a range of energies that possess no electron is called a **Forbidden gap**.

Banding of Discrete states and the Simplified Model

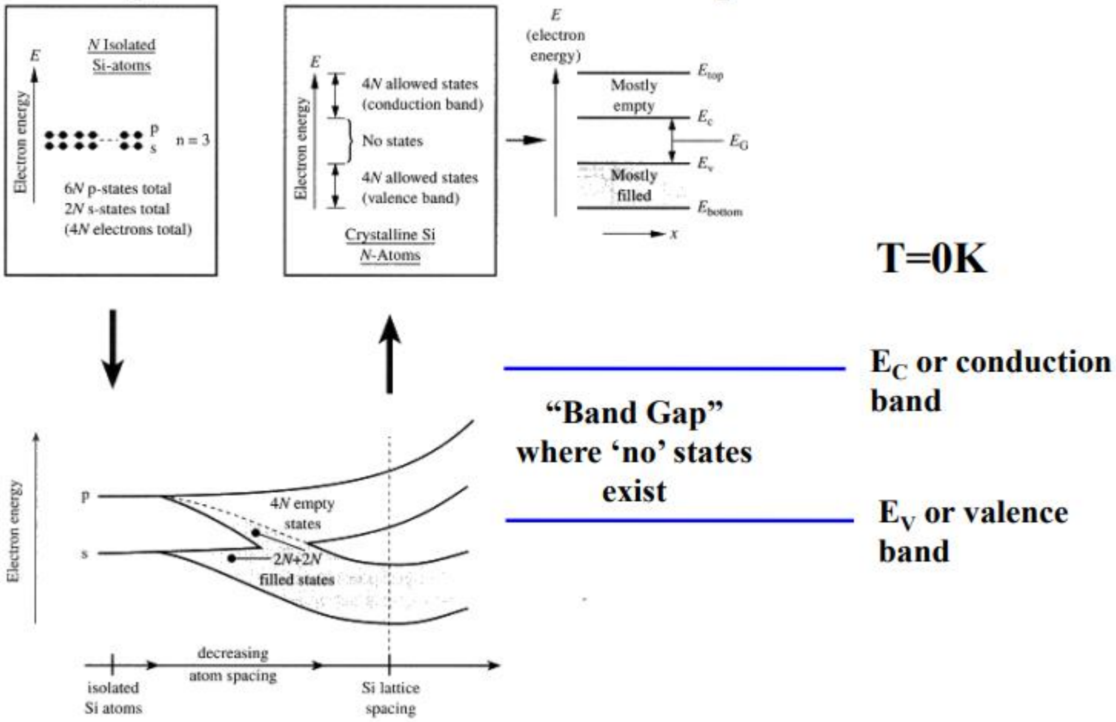
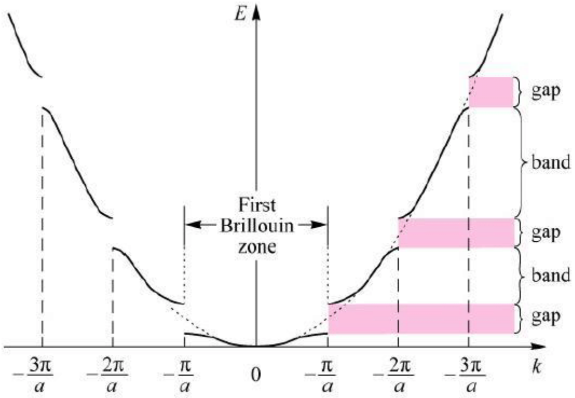


Figure 2.5 Conceptual development of the energy band model starting with N isolated Si atoms on the top left and concluding with a "dressed-up" version of the energy band model on the top right.

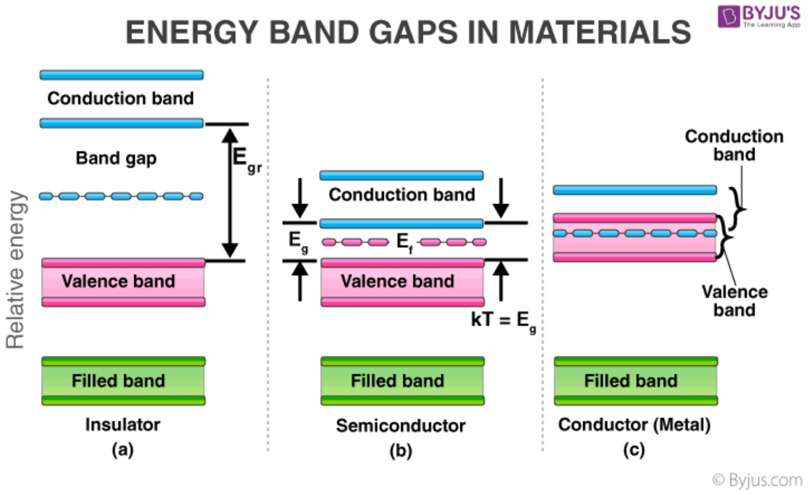
Since the electron energy levels are determined by the quantum numbers and, in a conglomeration of atoms of same type, the electron energy levels will separate into bands of energy levels. Such bands have energy widths typical of a given solid; however, the number of levels within the band is determined only by the number of atoms present. Recalling the Kronig-Penney model for a free electron in a solid, which resulted in an energy distribution as a function of *k*, the wave number, given by Fig. below



E-*k* plot from Kronig Penney Model

The allowed electronic energy states thus fall into bands, separated by regions known forbidden gaps. The number of available states in the band depends upon the number of atoms N present, and due to spin (± 1/2) of electrons, 2N electrons will be required to fill the first band, the two bands of importance for semiconductor terminology are the valance band and conduction band.

The lowest completely filled band is called the valence band the lowest partially filled band is called conduction band. In silicon and certain other diamond structures, for example, there is a quantum-mechanically forbidden zone between the valence and conduction bands. Metals have overlapping of band and therefore no forbidden zone exists at these higher energy levels. With reference to silicon, this forbidden gap occurs between 3S and 3P shells and has an energy span of 1.11 ev. In case of germanium, the gap is 0.72 ev and occurs between 4S and 4P shells. On the other hand, diamond is known to have a gap of 6 eV, located between 2S and 2P shells. With these ideas in mind, one can distinguish between insulators, semiconductors and metals (good conductors) pictorially shown below. In a metal, the uppermost energy band containing electrons is only partially filled, or a filled band overlaps an empty band (this is what allows some divalent metals to be good conductors, even though divalence is normally associated with good insulation). In semiconductors conductions happens as a result of thermally exciting electrons in the valence band of a crystal are able to jump the forbidden gap and enter the conduction band. This simultaneously creates an electron and hole called "pair". If an electric field were now applied, a net current would be observed. If a thermally excited electron gives up its energy and jumps back to the valence band, it will reunite with a hole in a process known as recombination.



Energy Band Diagram for Semiconductors, Conductors, and Insulators

Conduction Band (CB) and Valence Band (VB) in Semiconductors

Valence Band:

The energy band involving the energy levels of valence electrons is known as the valence band. It is the highest occupied energy band. When compared with insulators, the bandgap in semiconductors is smaller. It allows the electrons in the valence band to jump into the conduction band on receiving any external energy.

Conduction Band:

It is the lowest unoccupied band that includes the energy levels of positive (holes) or negative (free electrons) charge carriers. It has conducting electrons resulting in the flow of current. The conduction band possess high energy level and are generally empty. The conduction band in semiconductors accepts the electrons from the valence band.

What is Fermi Level in Semiconductors?

Fermi level (denoted by EF) is present between the valence and conduction bands. It is the highest occupied molecular orbital at absolute zero. The charge carriers in this state have their own quantum states and generally do not interact with each other. When the temperature rises above absolute zero, these charge carriers will begin to occupy states above Fermi level.

Typical Band Structure of Semiconductors

A semiconductor was defined as defined above as a solid in which the highest occupied energy band, the valence band, is completely full at T = 0K, but in which the gap above this band is also small, so that electrons may be excited thermally at room temperature from the valence band to the next-higher band, which is known as the conduction band. Generally speaking, the number of excited electrons is appreciable (at room temperature) whenever the energy gap E, is less than 3.5 eV. The substance may then be classified as a semiconductor. When the gap is larger, the number of electrons is negligible, and the substance is an insulator. When electrons are excited across the gap, the bottom of the conduction band (CB) is populated by electrons, and the top of the valence band (VB) by holes. As a result, both bands are now only partially full, and would carry a current if an electric field were applied. The conductivity of the semiconductor is small compared with the conductivities of metals of the small number of electrons and holes involved, but this conductivity is nonetheless sufficiently large for practical purposes. Only the CB and VB are of interest to us here, because only these two bands contribute to the current. Bands lower than the VB are completely full, and those higher than the CB completely empty, so that neither of these groups of bands contribute to the current; hence they may be ignored so far as semiconducting properties are concerned. In characterizing a semiconductor, therefore, we need describe only the CB and VB. The simplest band structure of a semiconductor is indicated in figure below. The energy of the CB has the form

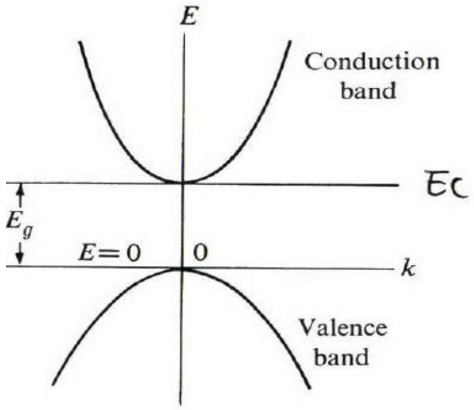
$$E_c(\mathbf{k}) = E_g + \frac{\hbar^2 k^2}{2m_e^*}$$

where k is the wave vector and m_e^* 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. We have used the standard band form to describe the CB, because we are primarily interested in the energy range close to the bottom of the band, since it is this range which contains most of the electrons. The energy of the VB may be written as

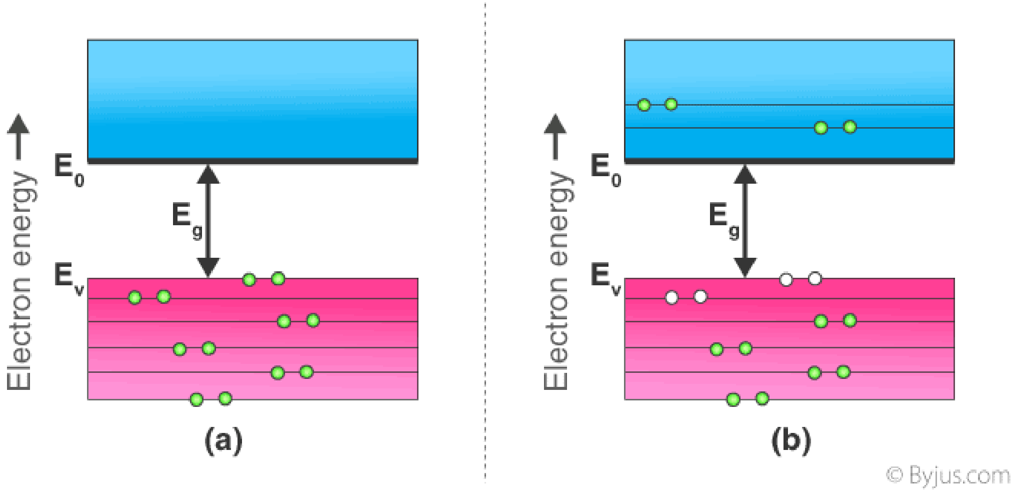
$$E_v(\mathbf{k}) = -\frac{\hbar^2 k^2}{2m_h^*}$$

where m_h^* is the effective mass of the hole. The VB is again represented by the standard inverted form because we are interested only in the region close to the top of the band, where most of the holes lie. The primary band-structure parameters are thus the electron and hole masses m_e and m_h (the asterisks have been dropped for convenience), and the band gap Ec. Note that the masses differ considerably from-and are often much smaller than-the freeelectron mass, and that the energy gaps range from 0.18 eV in InSb to 3.7 eV in ZnS.

The energy gap for a semiconductor varies with temperature, but the variation is usually slight. That a variation with temperature should exist at all can be appreciated from the fact that the crystal, when it is heated, experiences a volume expansion, and hence a change in its lattice constant. This, in turn, affects the band structure, whichis a sensitive function of the lattice constant. It also follows that the gap may be varied by applying pressure, as this too induces a change in the lattice constant. Studies of semiconductors under high pressure have, in fact, proved very helpful in elucidating some of their properties. The conduction and valence bands in semiconductors are related to the atomic states. When two hydrogen atoms are brought together to form a molecule, the atomic ls state splits into two states: a low-energy bonding state and a high-energy antibonding state. In solid hydrogen, these states broaden into bonding and antibonding energy bands, respectively. In like fashion, the valence and conduction bands in semiconductors are, respectively, the bonding and antibonding bands of the corresponding atomic valence states. Thus the VB and CB in Si, for example, result from the bonding and antibonding states of the hybrid $3s^13p^3$. Similar remarks apply to the bands in Ge, C, and other semiconductors.



Band structure in a semiconductor.



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(a) Intrinsic Semiconductor at T = 0 Kelvin, behaves like an insulator (b) At t>0, four thermally generated electron pairs