Classification of solid materials depending on the band gap

A **band gap** also called an **energy gap**, is an energy difference separating between the valence band (V.B) and conduction band (C.B) in a solid where no electronic states can exist. An imaginary level, which lies very close to the middle of the band gap, and depends on the density of electrons in (C.B) and the density of holes in (V.B), $E_F=(E_C+E_V)/2=E_g/2$, for the intrinsic semiconductor, is called **Fermi level**, see Figure 6.

The band structure of the metal is given in Figure 6 in which see the overlapping between the valance band (V.B) and conduction band (C.B). However, the insulator shows the large forbidden gap that separates the filled valence band from the vacant conduction band.

The band structure of the semiconductor shows the energy gap is relatively small.

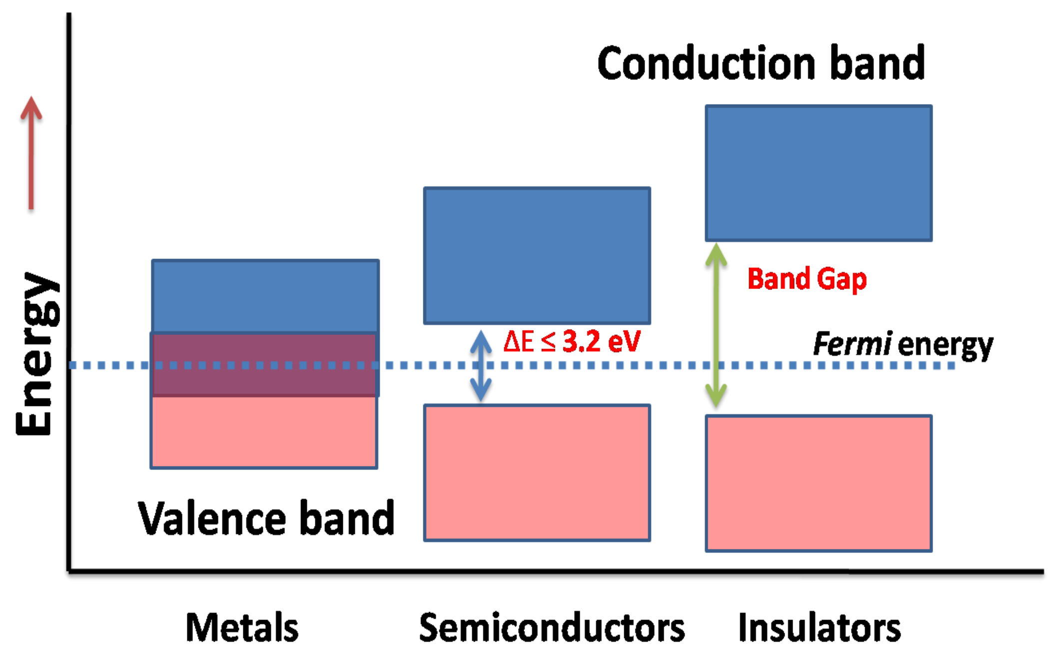

Figure 6. Conduction band (C.B) --- blue, Valence band (V.B) --- pink

Intrinsic semiconductor

It is a pure semiconductor (without impurity) in which the conduction band does not have electrons before heating, but after heating becomes the number of electrons (n) in the conduction band is equal to the number of holes (p) in the valence band so that (n=p), see Figure 7.

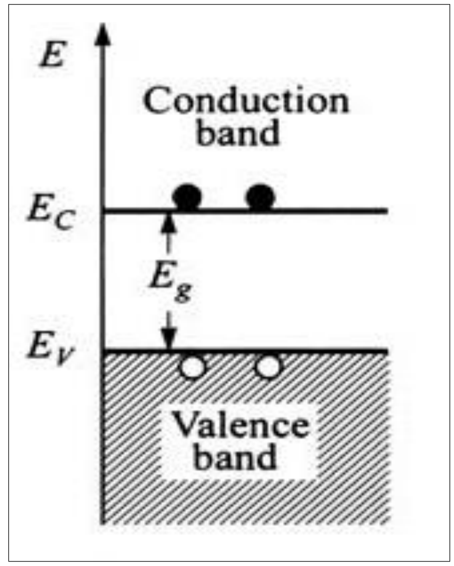

Figure 7.

Conduction in intrinsic semiconductors

Figure 8 shows the energy band diagram for an unexcited (no external energy, such as heat) atom in a pure silicon crystal. This condition occurs only at a temperature of (T=0K).

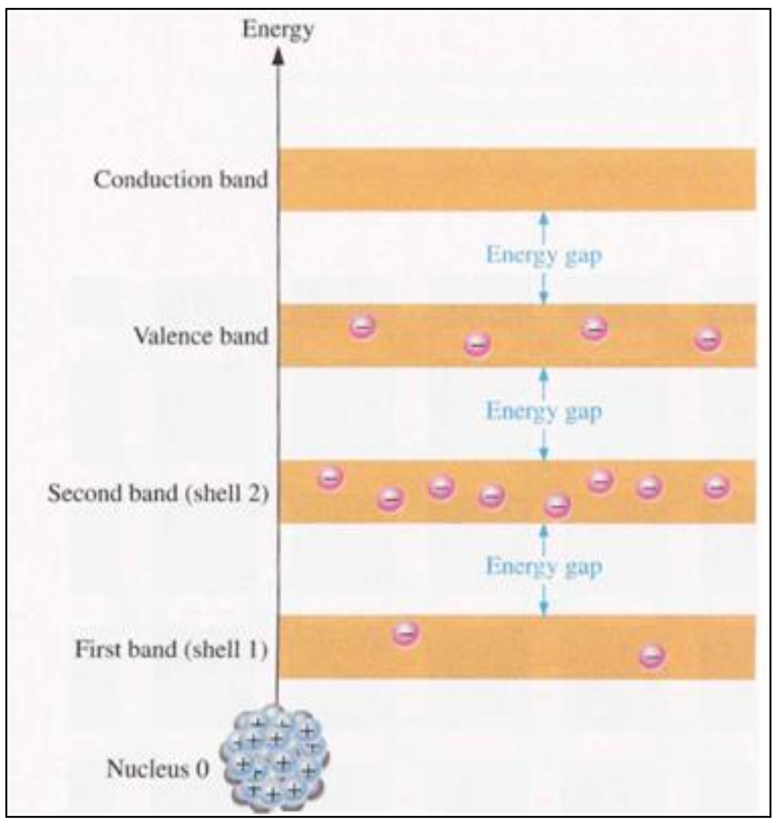

Figure 8.

At room temperature intrinsic (pure) silicon has sufficient heat (thermal) energy for some valence electrons to jump the gap from the (V.B) into the (C.B), becoming free electrons. Free electrons are also called conduction electrons. When an electron jumps to the conduction band, a vacancy is left in the valence band within the crystal. This vacancy is called ***a hole***. For every electron raised to the (C.B) by the external energy, there is one hole left in the (V.B), creating what is called ***an electron-hole pair***.

Recombination occurs when a conduction band electron loses energy and falls back into a hole in the valence band.

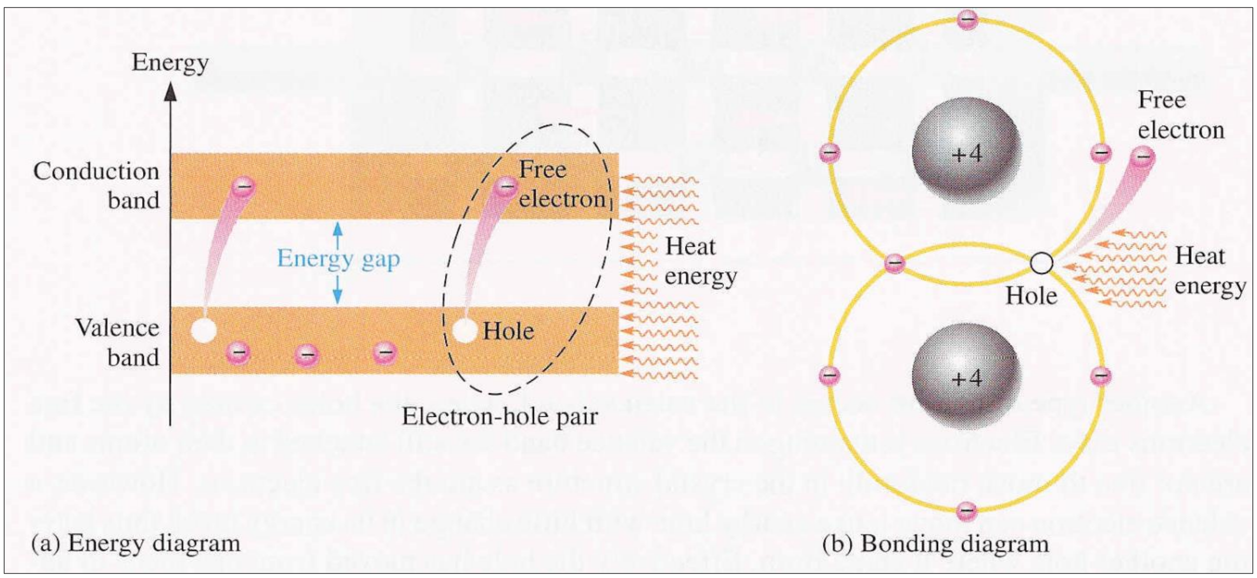

Figure 9.

The band gap of semiconductors

Figure 10 shows the energy levels of Ge, Si and GaAs. Each material has a specific band gap, which determines from the top energy level in the valence band to the lowest energy level in the conduction band, see the table below.

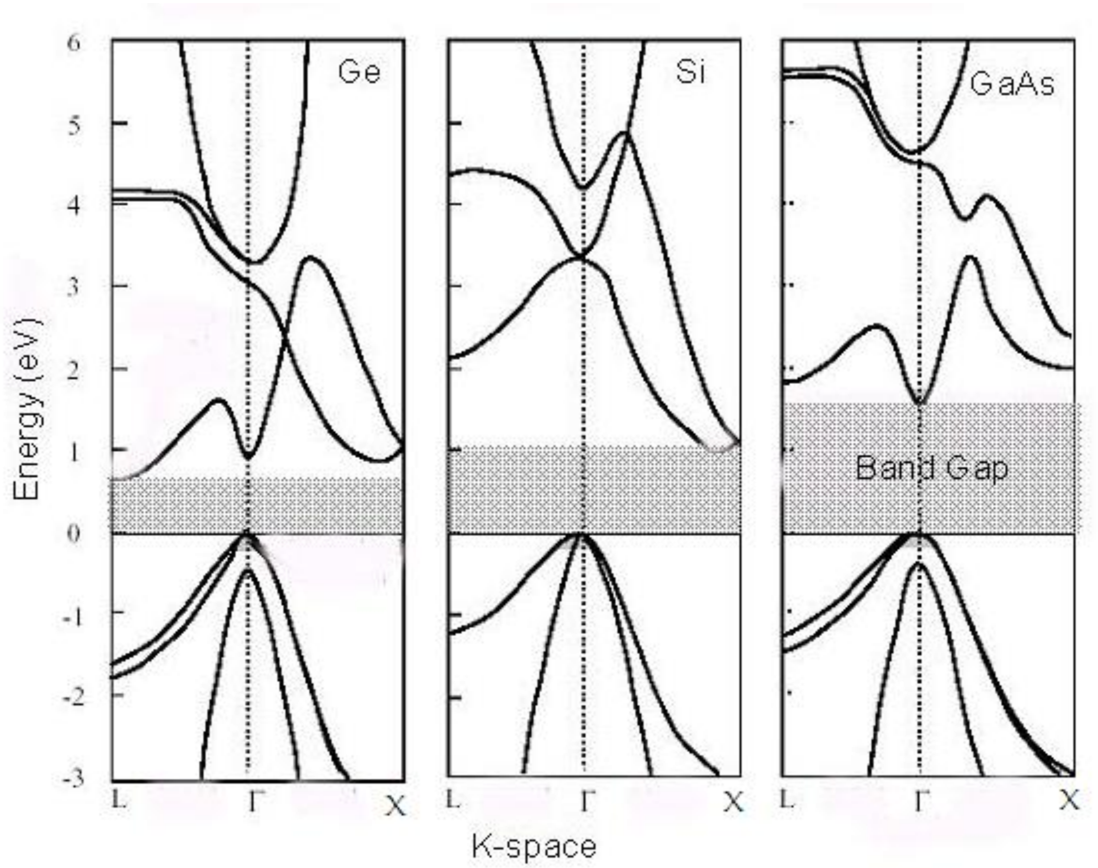

Figure 10.

Semiconductor	E_g (at 300K) in eV
Silicon (Si)	1.11
Germanium (Ge)	0.66
Gallium Arsenide (GaAs)	1.41
Indium phosphate (InP)	1.34
Zinc tellurite (ZnTe)	2.26
Cadmium Tellurite (CdTe)	1.43

The transition direction of the electron between the two energy levels for GaAs is different from Si. This means: semiconductor energy bands are classified into **direct** and **indirect** transitions.

The direct and indirect band gap

In a direct band gap for semiconductors, such as GaAs, an electron in the conduction band can fall to an empty state in the valence band, giving off the energy difference *Eg* as a photon of light. In an indirect band gap for semiconductors, such as Si, an electron in the conduction band cannot fall directly to the valence band but must undergo a momentum change as well as changing its energy, see Figure 11. In an indirect transition that involves a change in **k**, part of the energy is generally given up as heat to the lattice rather than as an emitted photon.

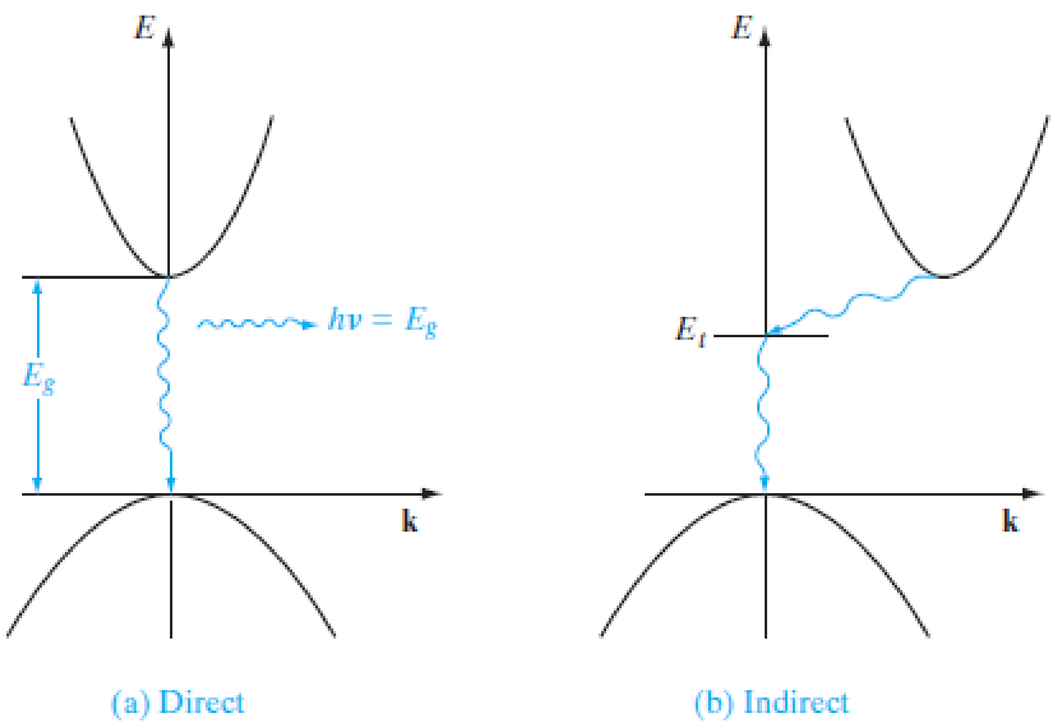

Figure 11.

Note: The indirect transition can occur due to some defect states (*E*t) within the band gap.

Why do we need this information?

This difference between direct and indirect band structures is very important for deciding which semiconductors can be used in devices requiring light output. For example, semiconductor light emitters and lasers generally must be made of materials capable of direct band-to-band transitions.

Band gap vs temperature

With the temperature, the band gap substantially varies, see Figure 12. The empirical relation of band gap vs temperature is

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

where α and β are constants.

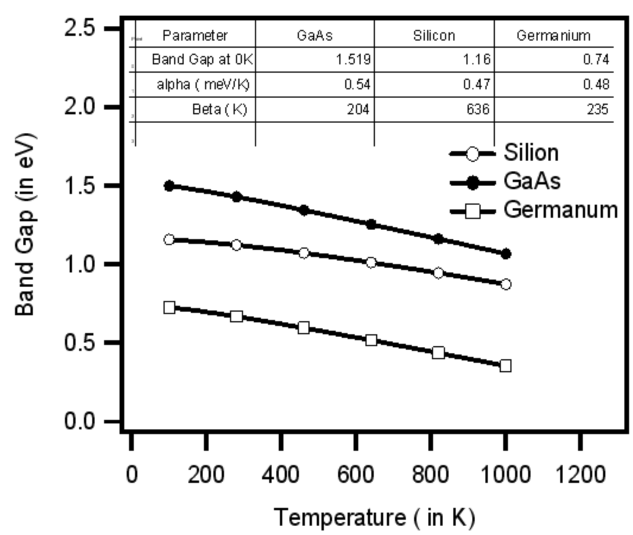

Figure 12.