(b) Direct and Indirect Semiconductors

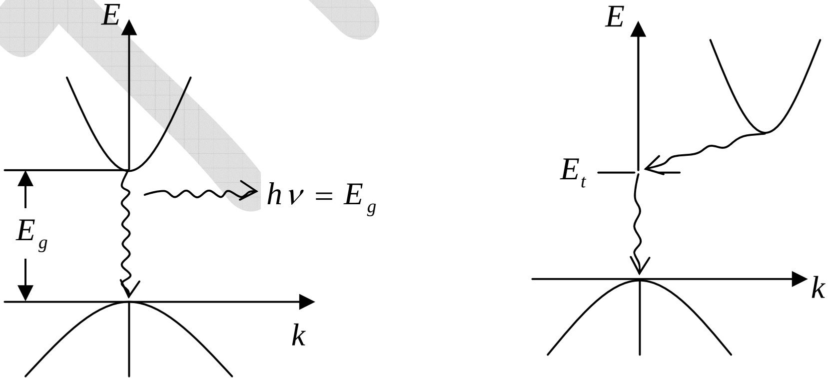
When quantitative calculations are made of band structures, a single electron is assumed to travel through a perfectly periodic lattice. The wave function of the electron is assumed to be in the form of a plane wave moving, for example, in the x-direction with propagation constant k, also called a wave vector. The space-dependent wave function for the electron is

$$\psi_k(x) = U(k_x, x)e^{ik_x x}$$

where the function $U(k_x, x)$ modulates the wave function according to the periodicity of the lattice.

In such a calculation, allowed values of energy can be plotted vs. the propagation constant k. Since the periodicity of most lattices is different in various directions, the (E, k) diagram must be plotted for the various crystal directions and the full relationship between E and k is a complex surface which should be visualized in three dimensions.

The band structure of $GaAs$ has a minimum in the conduction band and a maximum in the valence band for the same k value $(k = 0)$. On the other hand, Si has its valence band maximum at a different value of k than its conduction band minimum. Thus an electron making a smallest-energy transition from the conduction band to the valence band in $GaAs$ can do so without a change in k value; on the other hand a transition from the minimum point in the Si conduction band to the maximum point of the valence band requires some change in k. Thus there are two classes of semiconductor energy bands ***direct*** and ***indirect*** (Figure). We can show that an indirect transition involving a change in k requires a change of momentum for the electron.



(a) Direct

(b) Indirect

Figure: Direct and indirect electron transitions in semiconductors: (a) direct transition with accompanying photon emission; (b) indirect transition via a defect level.

In a direct semiconductor such as $GaAs$, an electron in the conduction band can fall to an empty state in the valence band, giving off the energy difference E_g as a photon of light. On the other hand, an electron in the conduction band minimum of an indirect semiconductor such as Si cannot fall directly to the valence band maximum but must undergo a momentum change as well as changing its energy. For example, it may go through some defect state $\left(E_t\right)$ within the band gap. In an indirect transition which involves a change in k, the energy is generally given up as heat to the lattice rather than as an emitted photon. 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 or of indirect materials with vertical transitions between defect states.