Bands in Intrinsic Semiconductors

The band structure of any real crystalline semiconductor is quite complicated and allows for different types of behavior. For example, silicon and germanium are said to be *indirect* band gap semiconductors and gallium arsenide a *direct* band gap semiconductor Fig (1). To be precise, in a direct band gap semiconductor an electron can be promoted from the valence band to the conduction band directly with no change in momentum, *e.g.*, by absorption of a photon. Physically, this occurs because of favorable alignment and curvature (or shape) of energy bands as constructed in a momentum representation. Conversely, in an indirect band gap semiconductor similar promotion of an electron from the valence band to the conduction band requires interaction with the crystal lattice in order to satisfy the principle of momentum conservation, *i.e.*, corresponding band alignment is unfavorable in “momentum space”. In passing, it is worthwhile to mention that distinction between direct and indirect band gap materials is of little importance for conventional electronic devices, but is technologically significant for optoelectronic devices, *e.g.*, light emitting diodes, laser diodes, *etc.*, which require direct band gap semiconductors for operation.

Even so, as asserted previously, for many (perhaps, most) practical situations detailed band structure is unimportant and can be greatly simplified into two aggregate bands, *viz.*, valence and conduction bands. Of course, just as in the case of atomic or molecular orbitals, electrons in a crystalline solid must satisfy the Pauli Exclusion Principle. Therefore, ignoring any effect of photo or thermal excitation, the valence band of a semiconductor can be regarded as completely filled and the conduction band as completely empty. Therefore, the conductivity of a pure semiconductor is expected to be quite low since mobility of electrons in the valence band is small. Naturally, this is merely a consequence of participation of the valence electrons in the bonding of the crystal lattice, which requires substantial localization of electron pairs between atomic nuclei. Nevertheless, as noted previously, conductivity of a pure semiconductor increases.

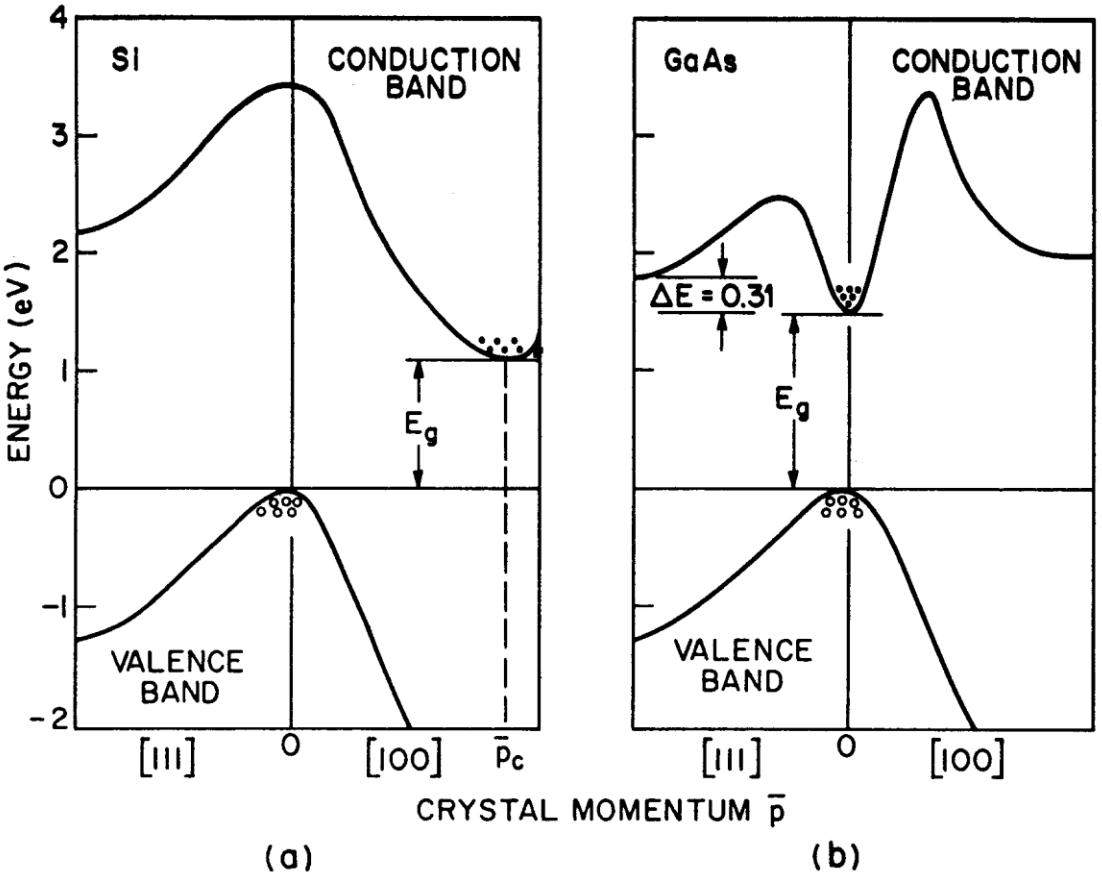

Figure 1. Energy band structures of Si and GaAs. Circles (o) indicate holes in the valence bands and dots (□) indicate electrons in the conductor bands.

Here, *f* (*E*), The probability that an electronic state with energy *E* is occupied by an electron is given by the Fermi-Dirac distribution function.

$$f(E) = \frac{1}{1 + \exp\left(\frac{E_i - E_f}{k_\beta T}\right)} \quad ------\rightarrow (3)$$

where E_F is the Fermi level, the energy at which the probability of occupation by an electron is exactly one-half. At room temperature, the intrinsic Fermi level lies very close to the middle of the bandgap.

The effective density of states in the conduction band N_C is equal to $2[2\pi m_n kT/h^2]^{3/2}$. Similarly, the effective density of states in the valence band N_V is $2[2\pi m_p kT/h^2]^{3/2}$. At room temperature, N_C for silicon is 2.8 x 10^{19} atoms/cm^3. For an intrinsic semiconductor, the number of electrons per unit volume in the conduction band is equal to the number of holes per unit volume in the valence band. That is, $n = p = n_i$ where *ni* is the intrinsic carrier density. Since $n = N_C\exp\{-$

$(E_C-E_F)/kT\}$ and $p = N_V\exp\{-(E_F-E_V)/kT\}$, where n is the electron density and p is the hole density, $np = n_i^2 = N_CN_V\exp\{(E_V-E_C)/kT\} = N_CN_V\exp\{-E_g/kT\}$. Therefore, is the probability that an electron state of energy, E, is occupied. The quantity, E_F, is called *Fermi energy* and defines a characteristic energy for which it is equally likely that an electron state of precisely that energy will be either vacant or occupied, *i.e.*, the state has an occupation probability of exactly one half. Clearly, any band state must be either occupied or vacant and, moreover, the approximate symmetric behavior of electrons and holes implies that a vacant electronic state can just as well be regarded as an occupied *hole state* and vice versa. Accordingly, it follows that the occupation probability for holes, *fh*(□*E*), is trivially related to *f*(*E*) by the simple formula:

$$f(-E) = \frac{1}{1 + \exp\left(\frac{E_f - E_i}{k_\beta T}\right)} \quad ------\rightarrow (3)$$

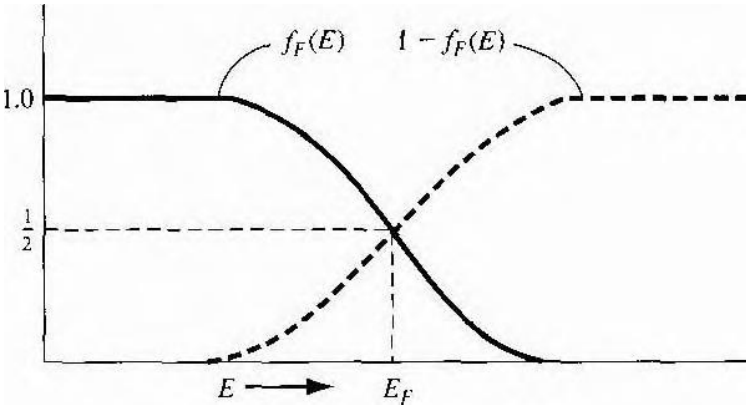

Figure 2. The probability of a state being occupy f(E), and the probability of a state