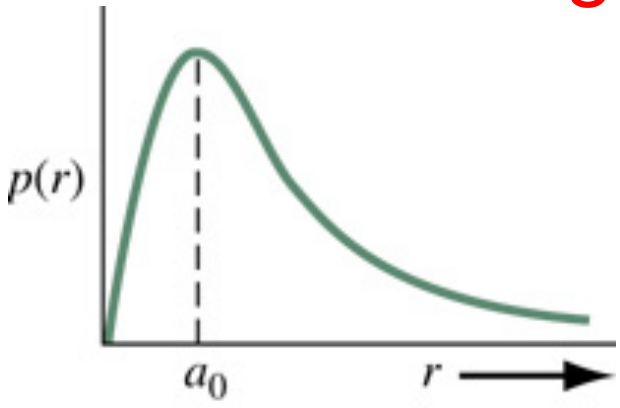
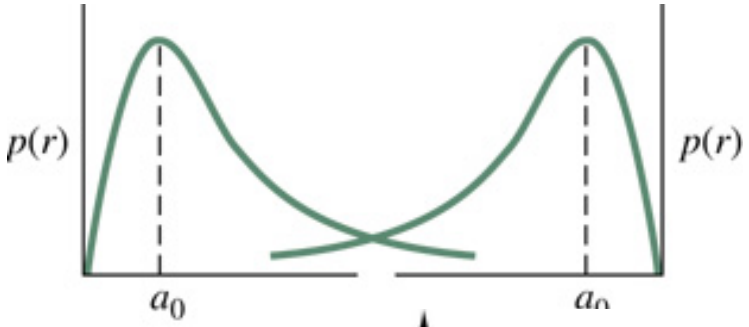
Quantum Theory of Solids

Ch. 3, Neamen

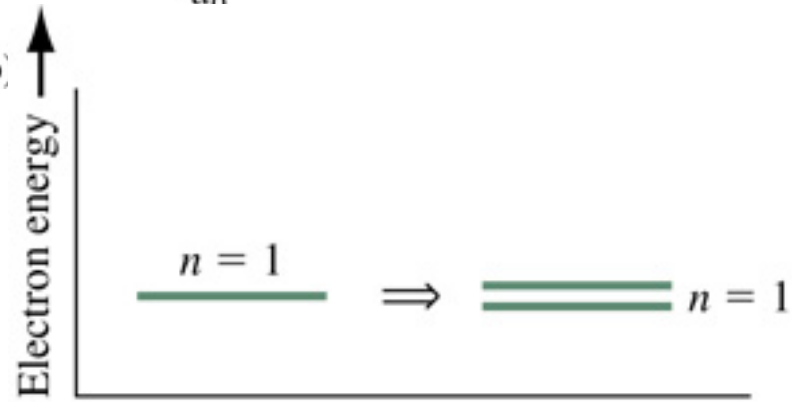
Bring two atoms together



(a)

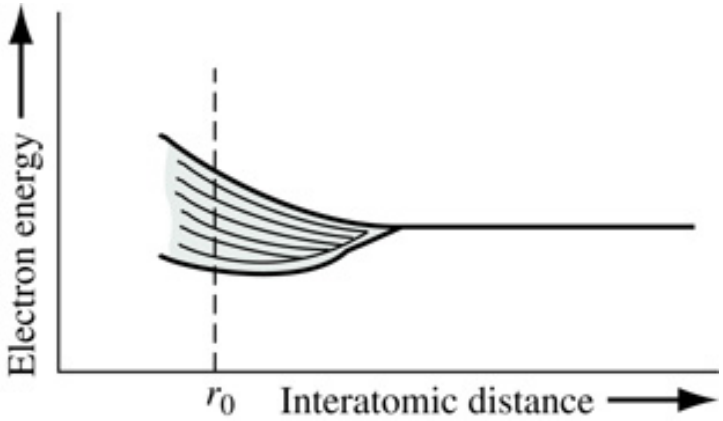


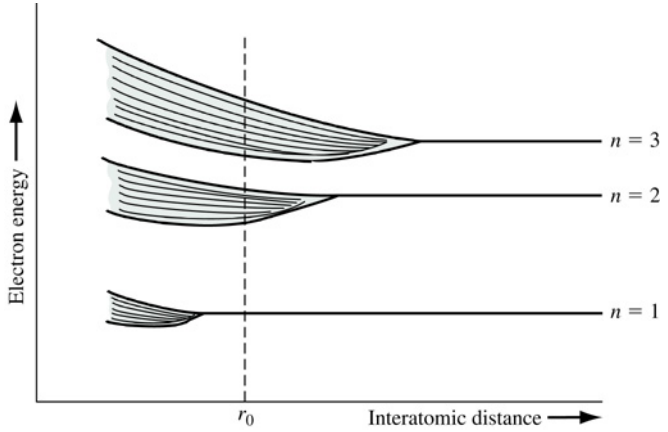
(b)

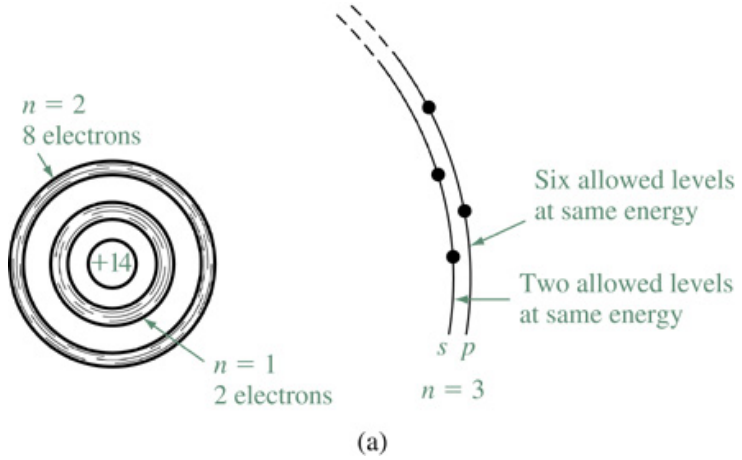


(c)

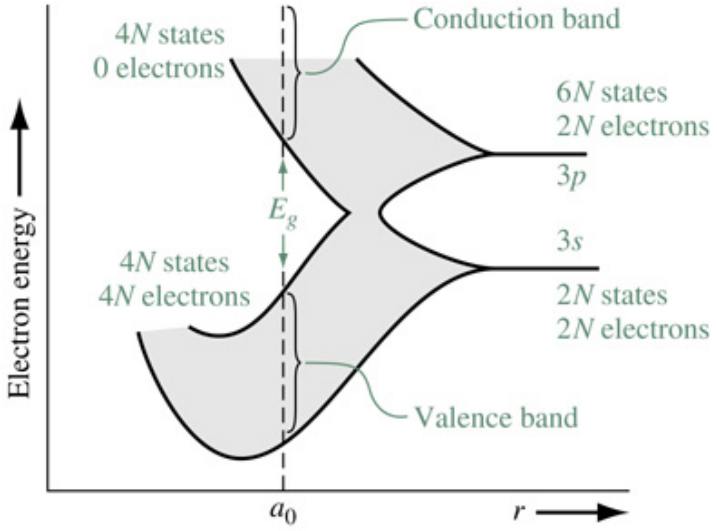
N Silicon Atoms





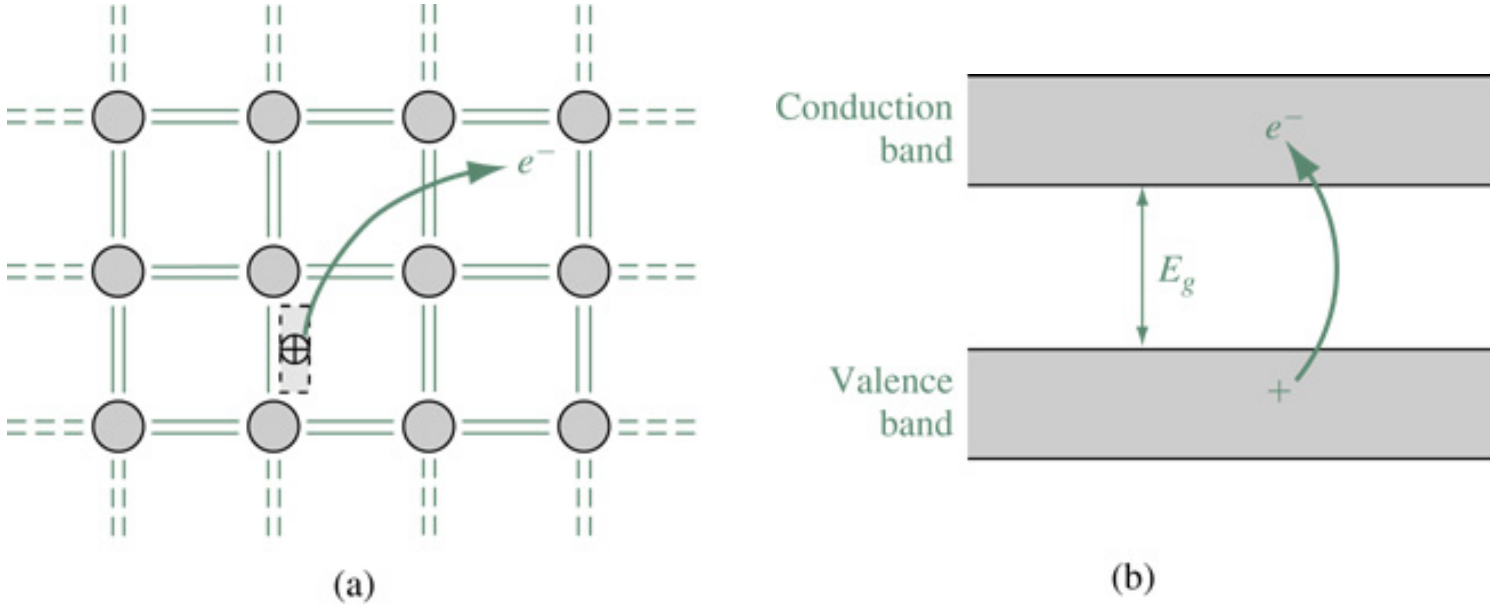


(a)

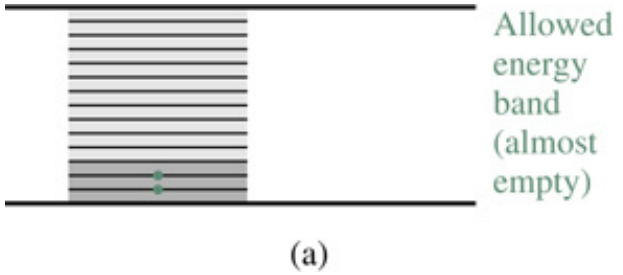


(b)

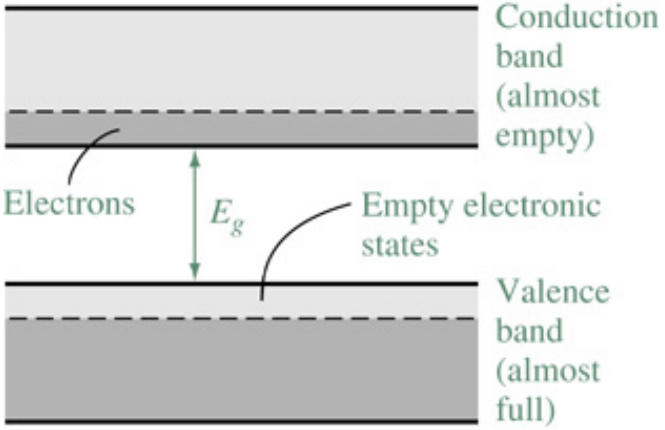
Breaking a covalent bond needs E_g energy
Produces an electron hole pair (EHP).
These are intrinsic carriers
$n=p=n_i$



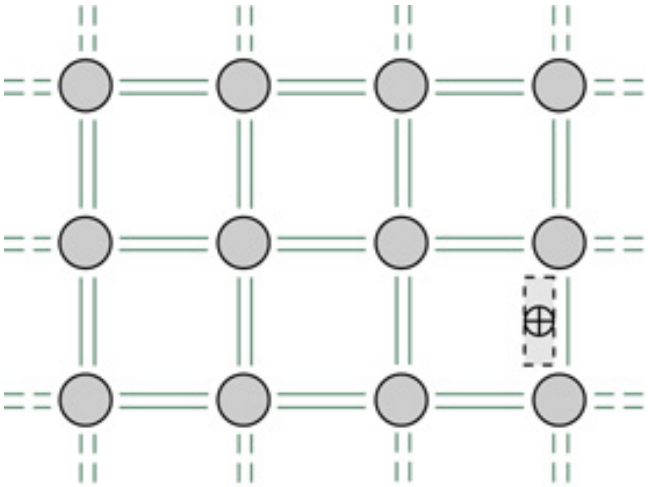
Mostly empty conduction band
Mostly filled valence band



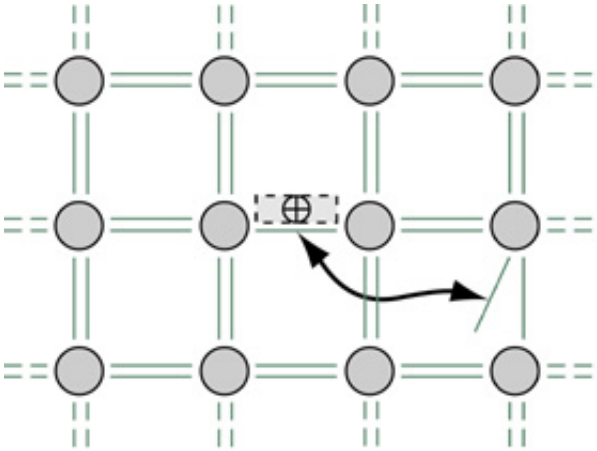
(a)



(c)



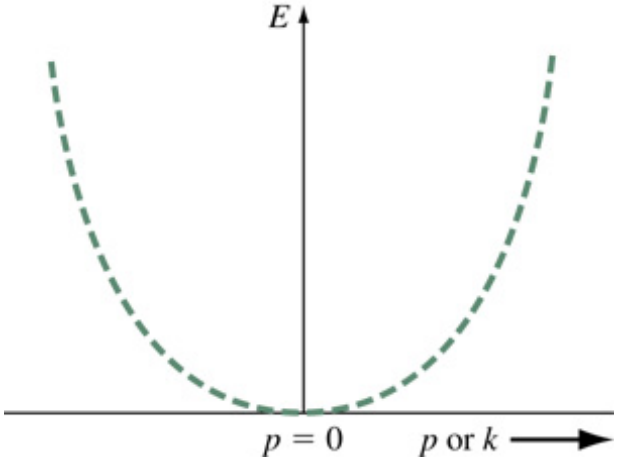
(c)



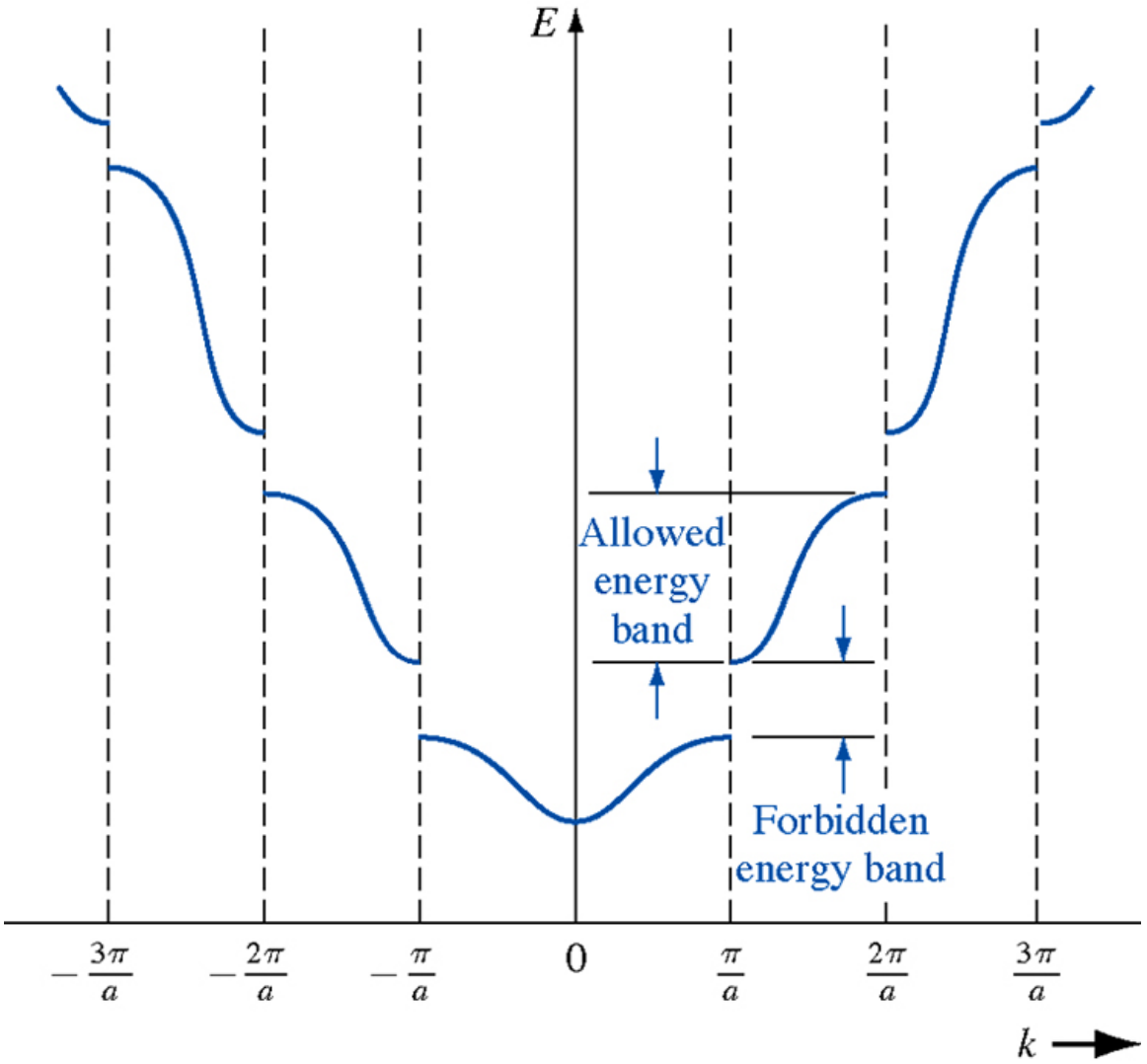
(b)

E-K diagram of free electrons

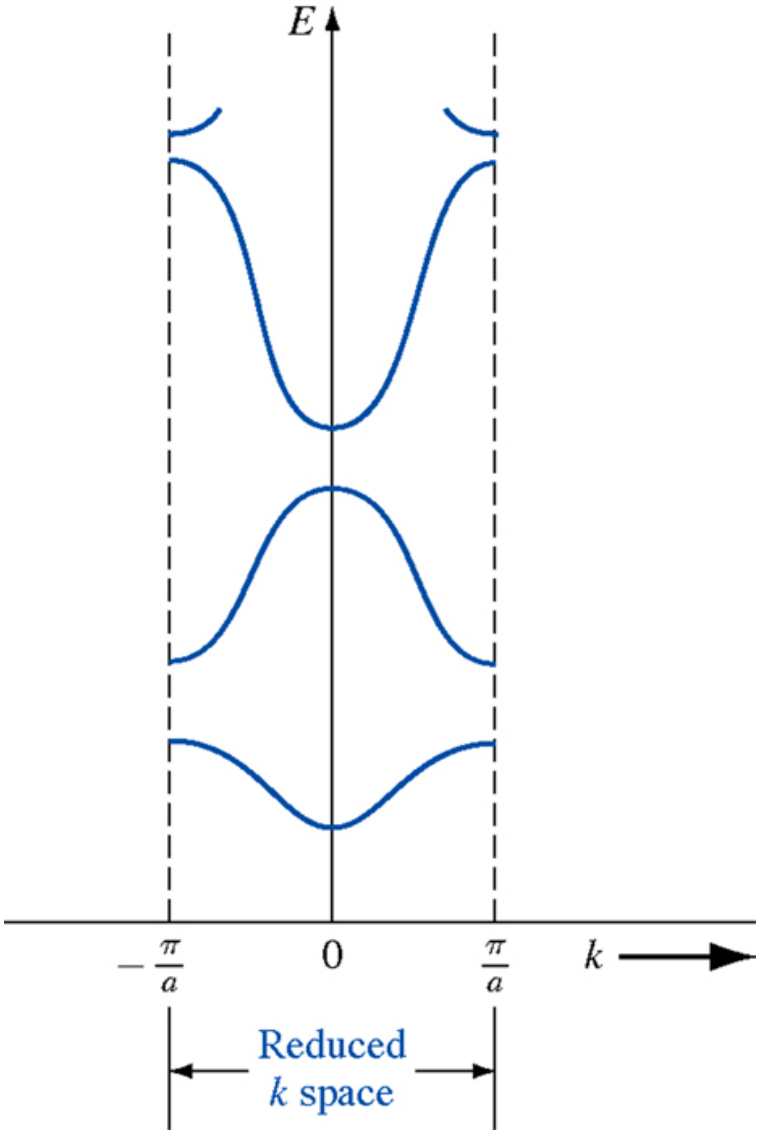
$$E = \frac{\hbar^2 k^2}{2m_0}$$



In a periodic structure, such as crystals, E-K changes to Energy Bands Boundaries are “Brillouin Zones”

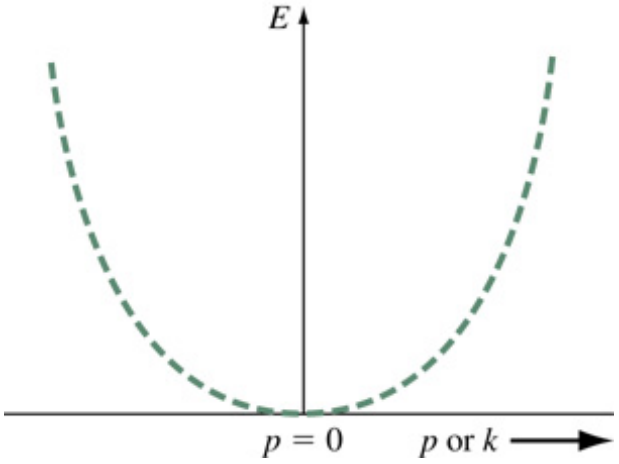


Usually drawn in Reduced Zone scheme

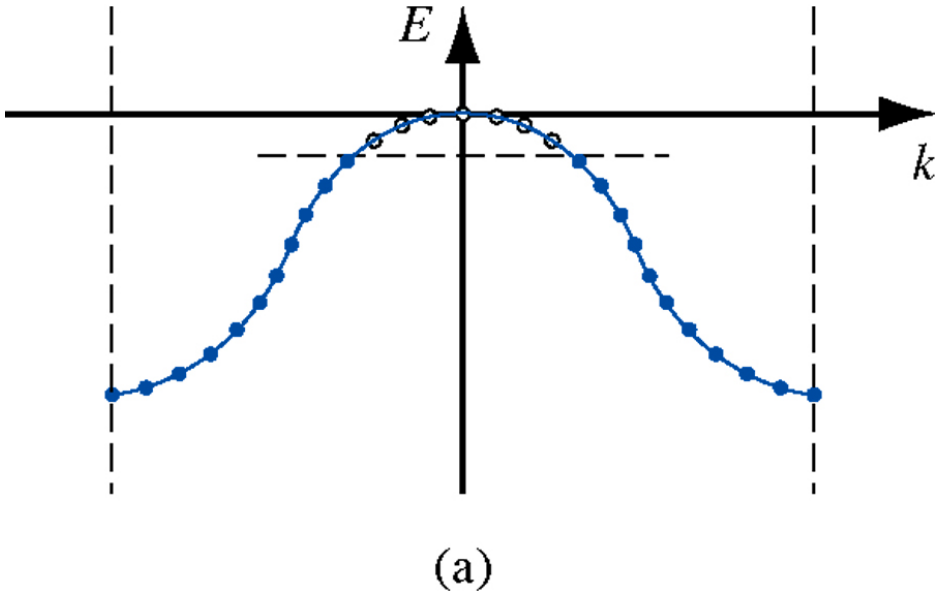


We can simplify this by introducing Effective Mass, m*

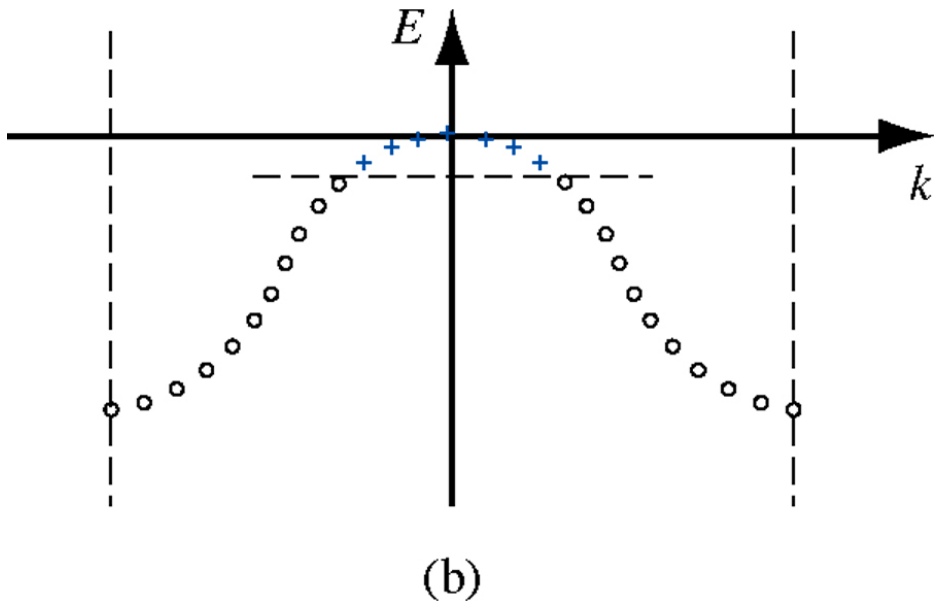
$$E = \frac{\hbar^2 k^2}{2m^*}$$



Empty States in Valence band = Holes

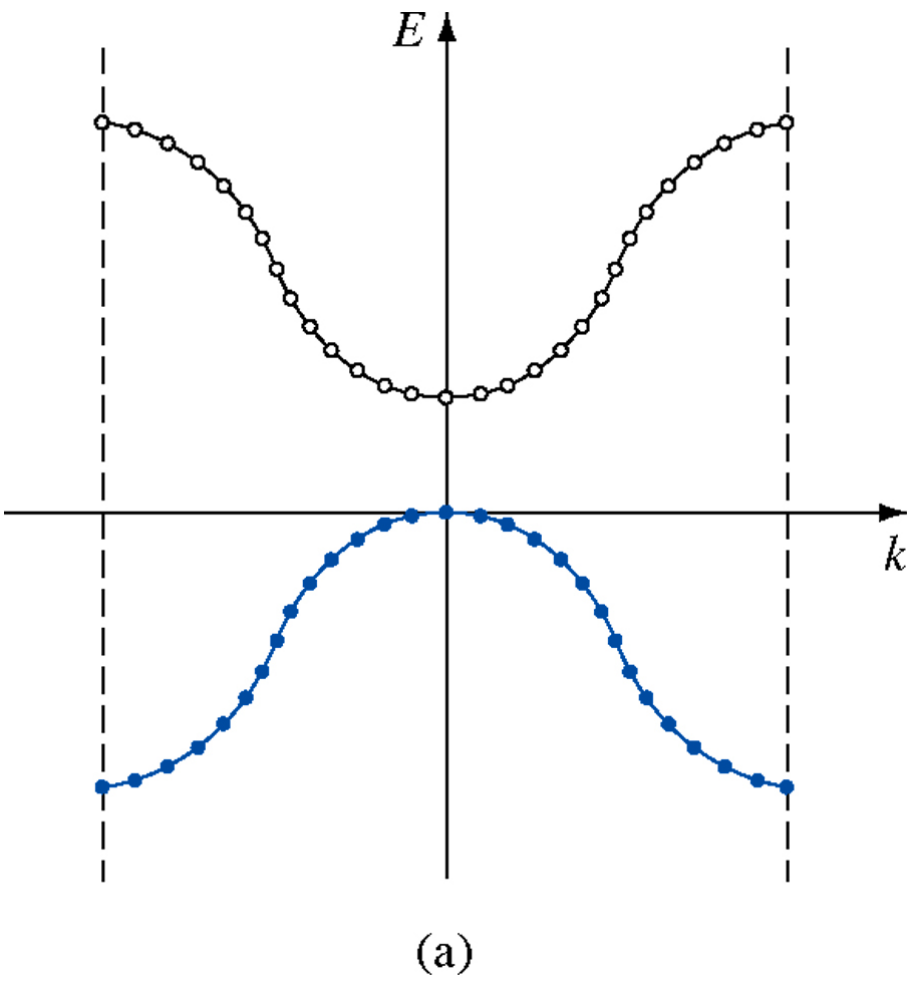


(a)

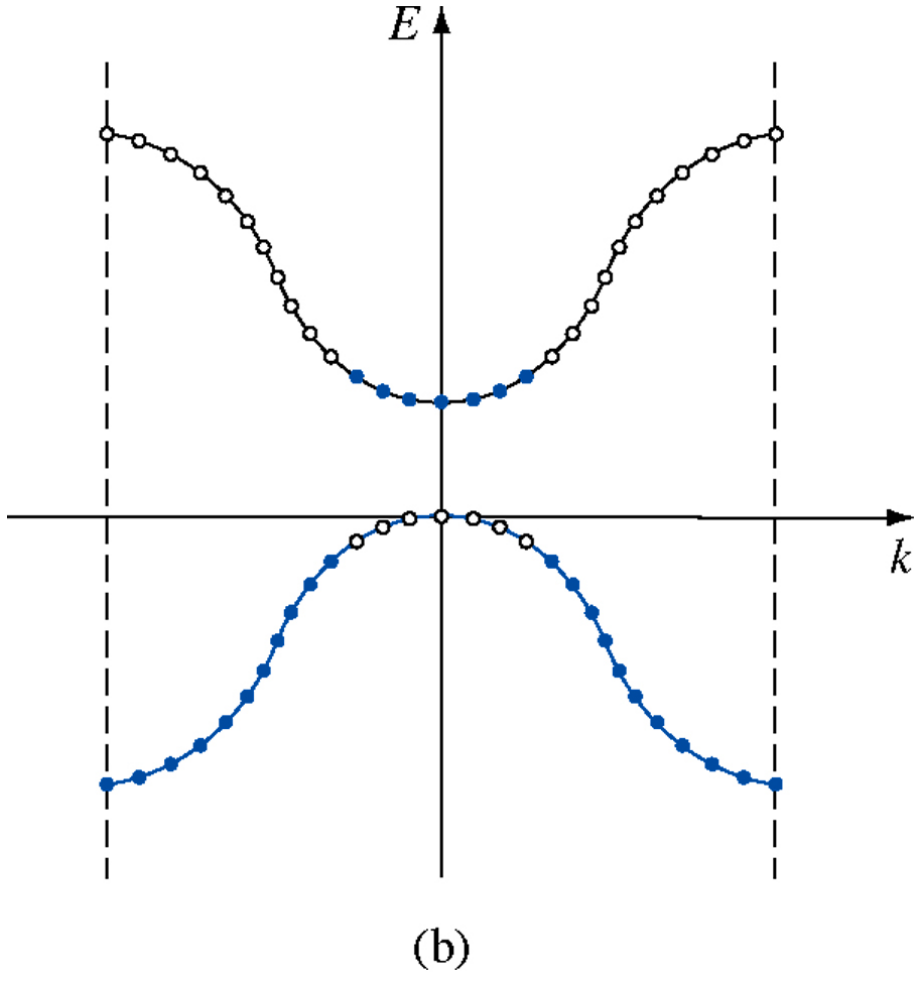


(b)

Electrons in semiconductors

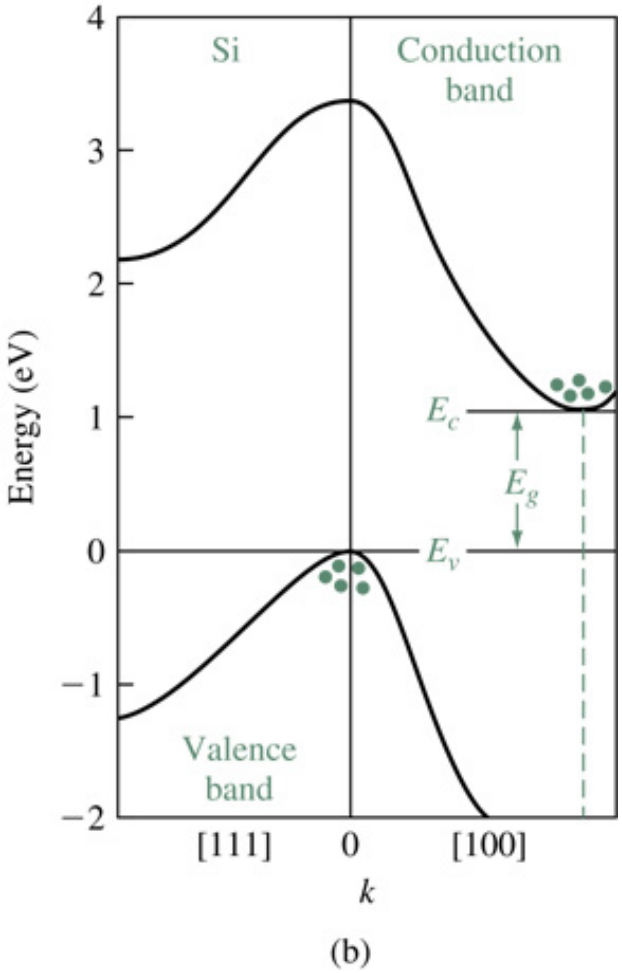


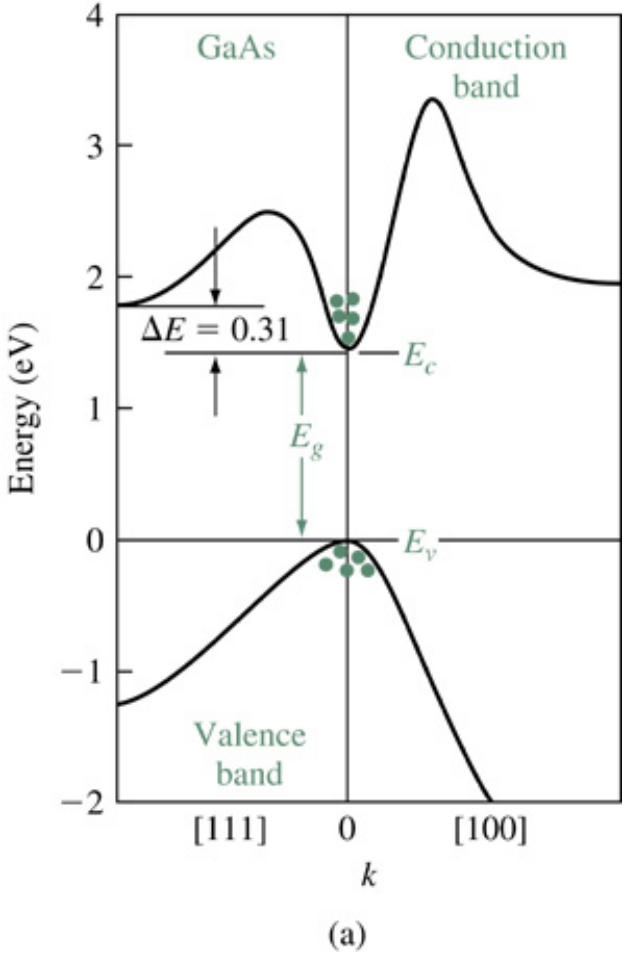
(a)



(b)

Silicon is indirect, GaAs is direct





BANDSTRUCTURE OF SEMICONDUCTORS

The *k*-vector for the electrons in a crystal is limited to a space called the Brillouin zone. The figure shows the Brillouin zone for the fcc lattice relevant for most semiconductors. The values and notations of certain important *k*-points are also shown. Most semiconductors have bandedges of allowed bands at one of these points.

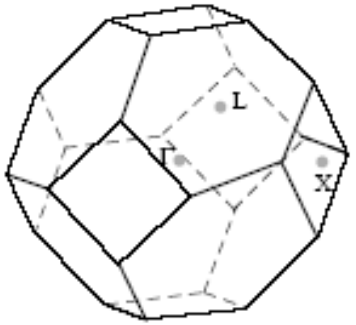
IMPORTANT HIGH SYMMETRY POINTS

Γ point: $k_x = 0 = k_y = k_z$

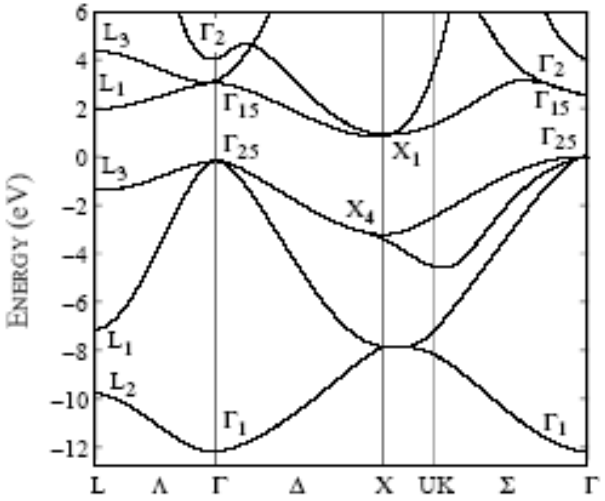
X point: $k_x = \frac{2\pi}{a}$; $k_y = k_z = 0$

L point: $k_x = k_y = k_z = \frac{\pi}{a}$

a = lattice constant (cube edge)

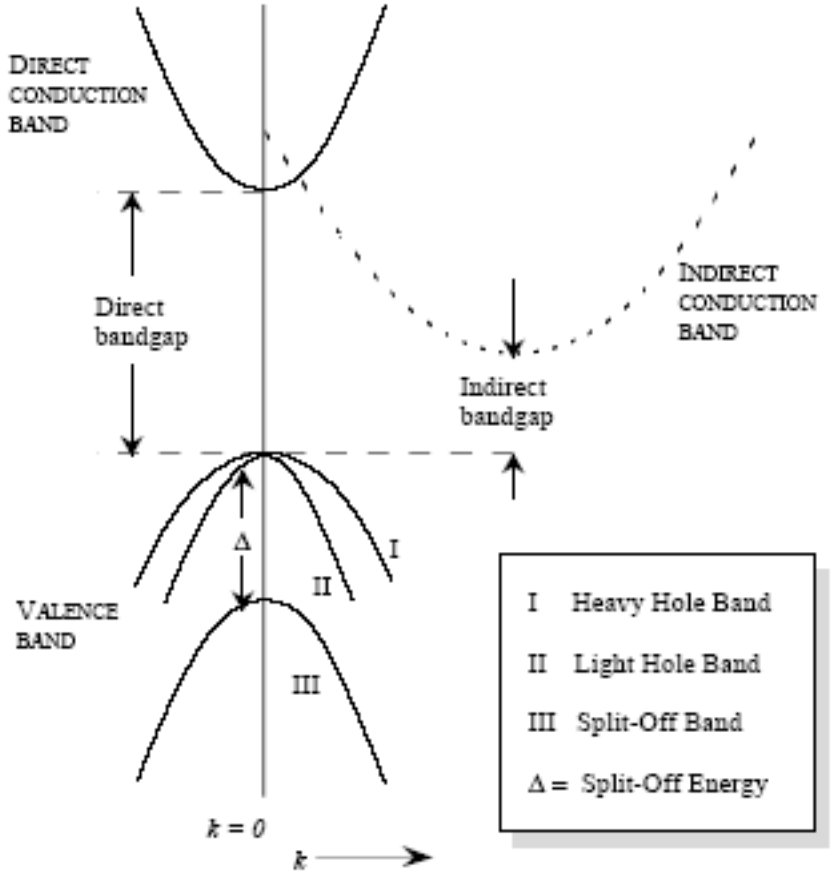


A TYPICAL BANDSTRUCTURE: Si



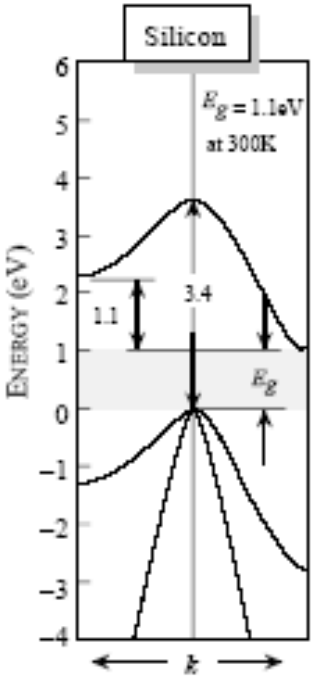
BANDSTRUCTURE NEAR BANDEDGES

Behavior of electrons near the bandedges determines most device properties. Near the bandedges the electrons can be described by simple effective mass pictures, i.e., the electrons behave as if they are in free space except their masses are m^*.

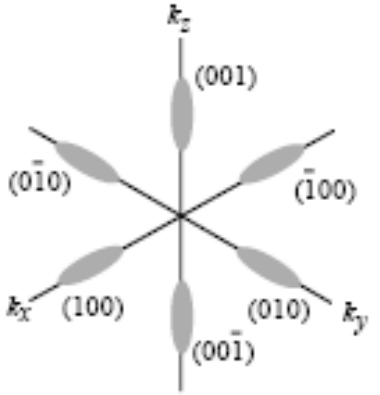


Schematic of the valence band, direct bandgap, and indirect bandgap conduction bands. The conduction band of the direct gap semiconductor is shown in the solid line, while the conduction band of the indirect semiconductor is shown in the dashed line. The curves I, II, and III in the valence band are called *heavy hole, light hole, and split-off hole states*, respectively.

A closer look at Si Energy Band Diagram



(a)



Six equivalent valleys at conduction bandedge

$$E_g = 1.17 - \frac{4.37 \times 10^{-4}\, T^2}{T - 636}\ (\text{eV}) \qquad T = \text{Temperature in K}$$

(b)

- Indirect gap material $\Rightarrow$ weak optical transitions, cannot be used to produce lasers.
- Valleys along the x-axis and $-x$-axis: $k_{0x} = \frac{2\pi}{a}(0.85,0,0)$ and $k_{0x} = \frac{2\pi}{a}(-0.85,0,0)$:

$$E(k) = E_c + \frac{\hbar^2}{2}\left[\frac{(k_x - k_{0x})^2}{m_l^*} + \frac{k_y^2 + k_z^2}{m_t^*}\right]; \; m_l = 0.98\, m_0; \; m_t = 0.19\, m_0$$

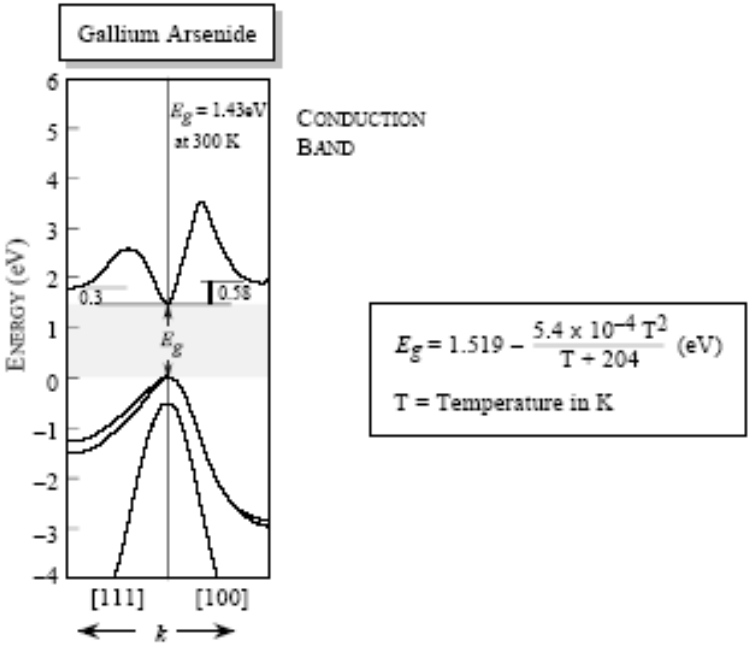
  similar E-k relations for other 4 valleys.

- Density of states mass = 1.08 m_0 (6 valleys included).
- Heavy hole mass: 0.49 m_0 ; light hole mass: 0.16 m_0.
- Intrinsic carrier concentration at 300 K: 1.5×10^{10} cm^{-3}.

And GaAs Energy Band Diagram

BANDSTRUCTURE: GaAs

The bandgap at 0 K is 1.51 eV and at 300 K it is 1.43 eV. The bottom of the conductionband is at $k = (0,0,0)$, i.e., the G-point. The upper conduction band valleys are at the L-point.



$$E_g = 1.519 - \frac{5.4 \times 10^{-4}\, T^2}{T + 204} \text{ (eV)}$$

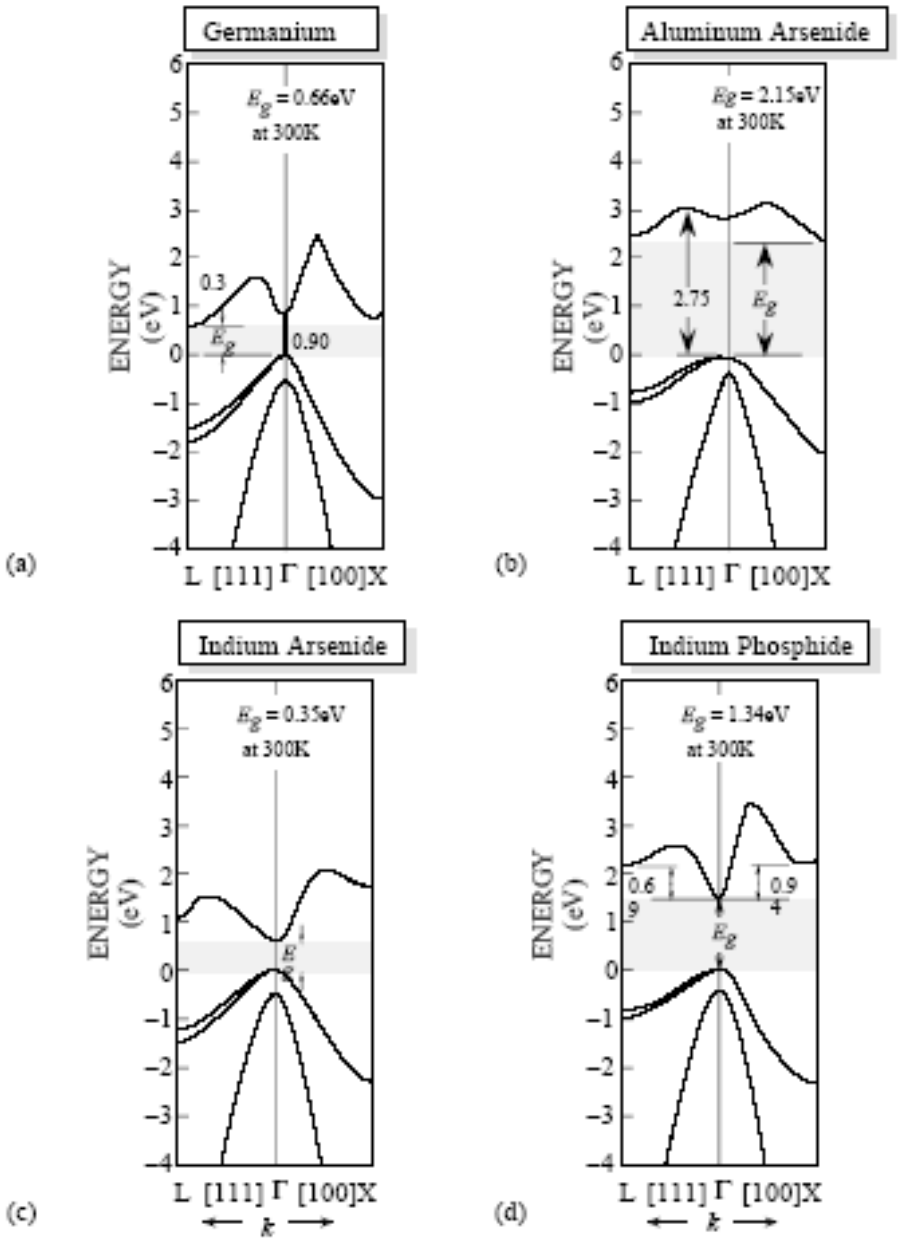
T = Temperature in K

CONDUCTION BAND:
- Electron mass is light. $m^* = 0.067\, m_0$
- Upper valley mass is large. $m^* = 0.25\, m_0$ results in negative differential resistance at higher fields.
- Material is direct bandgap and has strong optical transistions ⇒ can be used for light emission.

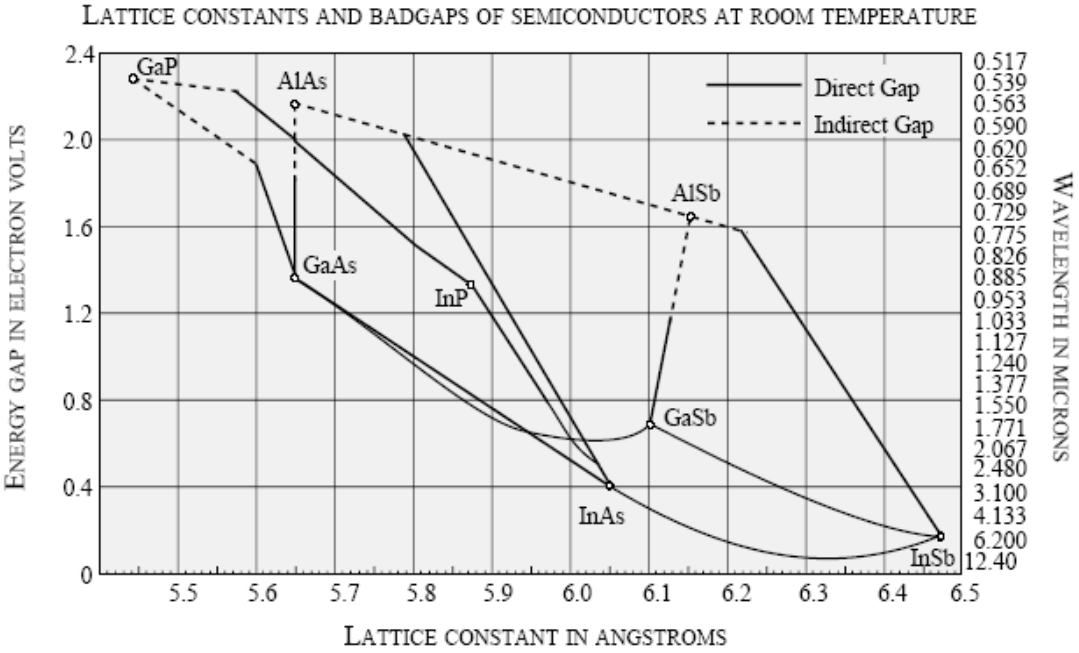
VALENCE BAND:
- Heavy hole mass: 0.45 m_0; light hole mass = 0.08 m_0.

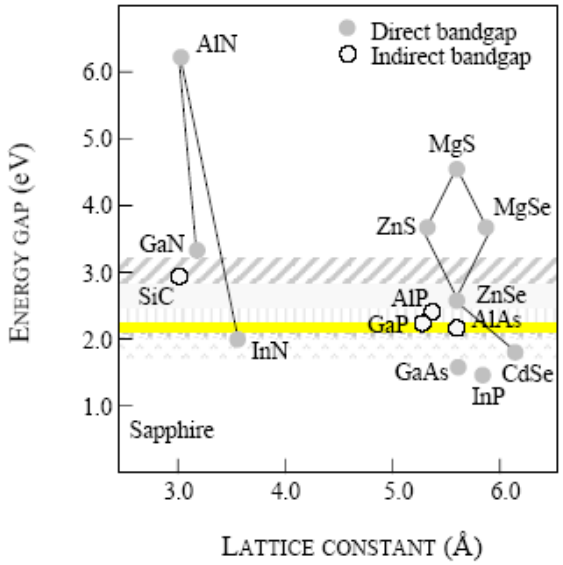
Intrinsic carrier concentration at 300 = 1.84×10^6 cm^{-3}.

Ge, AlAs, InAs, InP Energy Band Diagram

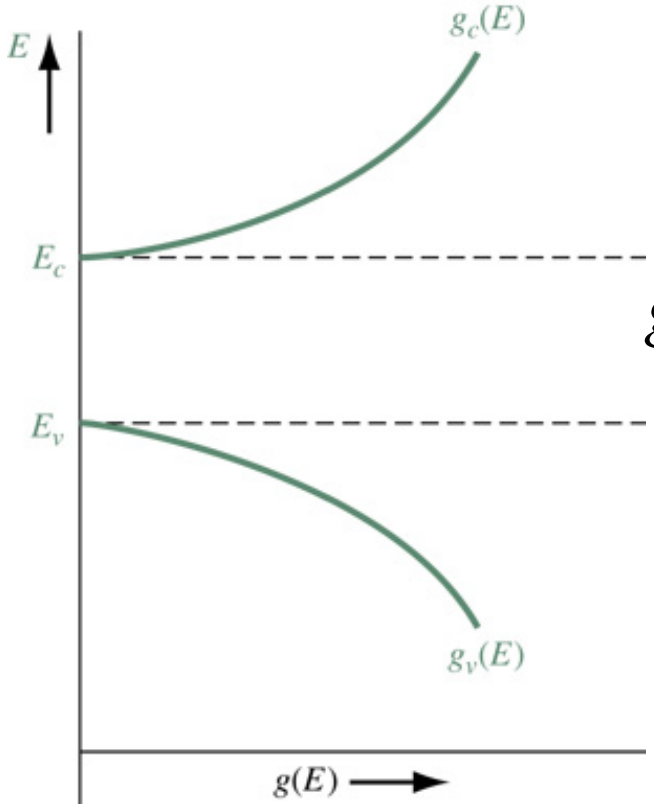


Lattice Constant and Band Gap





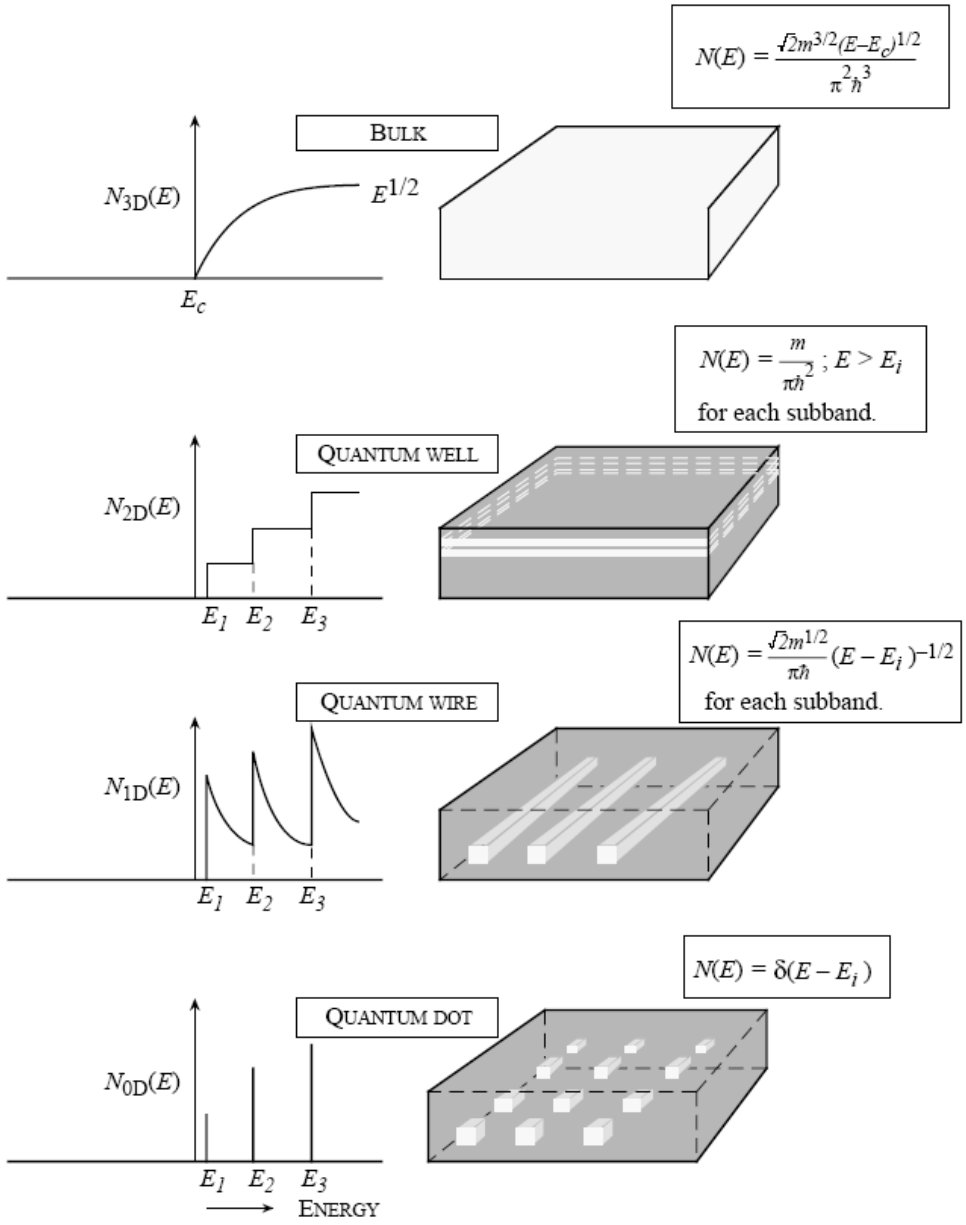
Density of States Function



$$g_{C,V}(E) = \frac{4\pi(2m^*_{n,p})^{3/2}}{h^3}\sqrt{E - E_{c,v}}$$

Low-dimensional structures: Density of states

One of the most important motivations for low-dimensional systems is the ability they offer to modiy the density of statees.



Fermi Function

- Probability of finding an electron at energy level E is

$$f(E) = \frac{1}{1 + \exp\left(\frac{E - E_F}{KT}\right)}$$

- where E_F is the Fermi level (or chemical potential, or electrochemical potential)