Semiconductor

Band theory of solids

There are usually two approaches to understand the origin of band theory associated with solids. One is the “nearly free electron model” and the other “tight-binding model”.

1) Nearly free electron model:
In the nearly free electron approximation, interactions between electrons are completely ignored. This model allows use of Bloch's Theorem which states that electrons in a periodic potential have wavefunctions and energies which are periodic in wavevector up to a constant phase shift between neighboring reciprocal lattice vectors.

2) Tight-binding model
The opposite extreme to the nearly-free electron model assumes the electrons in the crystal behave much like an assembly of constituent atoms.

Bloch functions

A **Bloch wave** or **Bloch state**, named after Felix Bloch, is the wavefunction of a particle (usually, an electron) placed in a periodic potential. It consists of the product of a plane wave envelope function and a periodic function (*periodic Bloch function*) $u_{n\mathbf{k}}(r)$ which has the same periodicity as the potential:

$$\psi_{n\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} u_{n\mathbf{k}}(\mathbf{r})$$

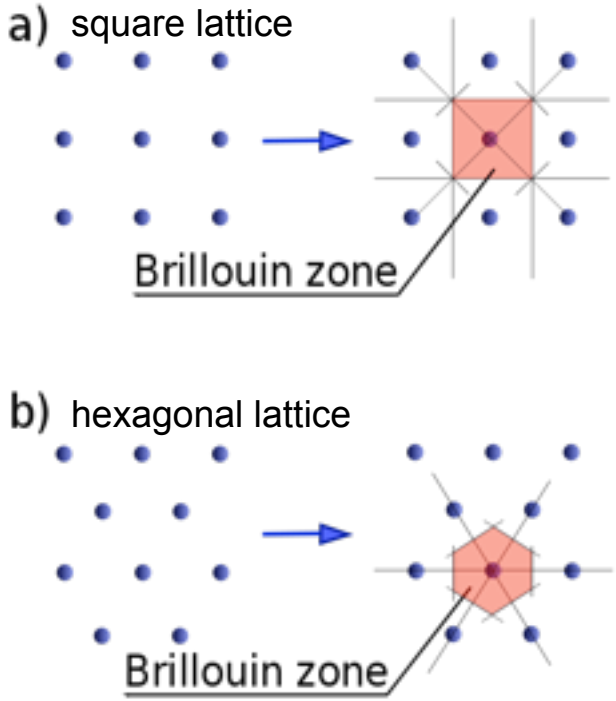
$$u_{n\mathbf{k}}(\mathbf{r}+\mathbf{T}) = u_{n\mathbf{k}}(\mathbf{r})$$

The corresponding energy eigenvalue is

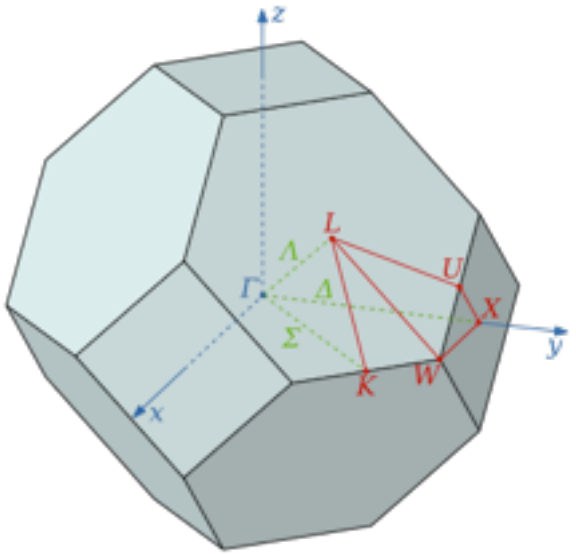
$$\epsilon_n(\mathbf{k}) = \epsilon_n(\mathbf{k} + \mathbf{G}).$$

Brillouin zone

The first **Brillouin zone** is a uniquely defined **primitive cell** in **reciprocal space**.



First Brillouin zone of FCC lattice showing symmetry labels for high symmetry lines and points

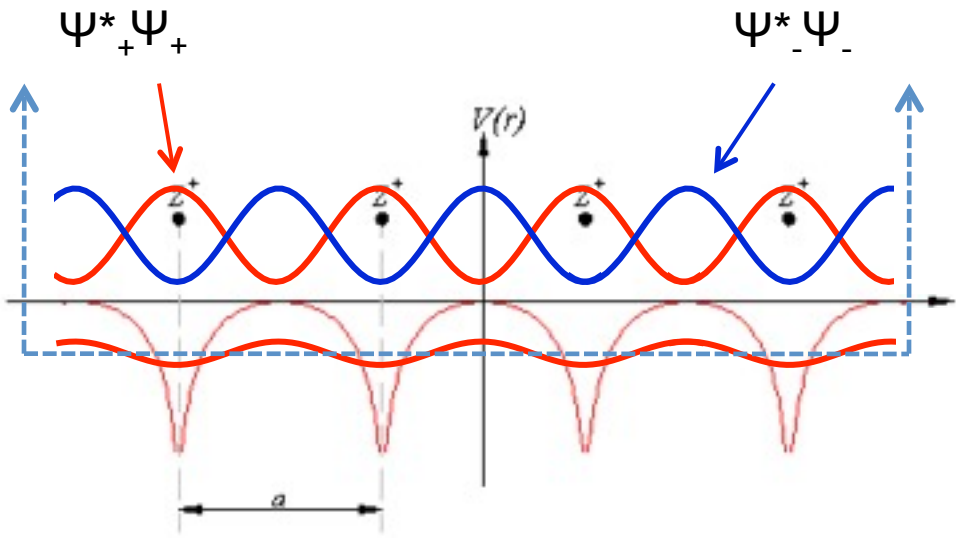


K	Middle of an edge joining two hexagonal faces
L	Center of a hexagonal face
U	Middle of an edge joining a hexagonal and a
W	Corner point
X	Center of a square face

At k = ± π/*a*

$$\Psi_+(x) = e^{ikx} + e^{-ikx} = 2cos(\pi x/a)$$

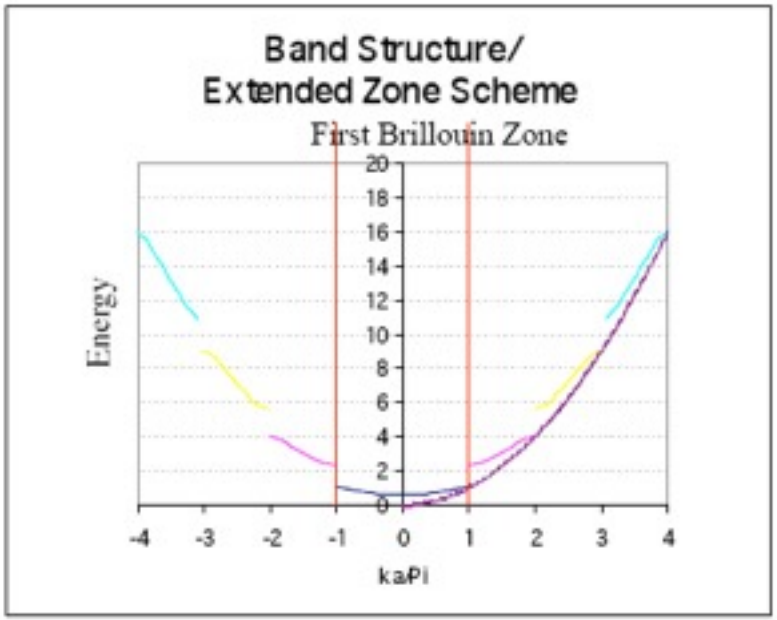
$$\Psi_-(x) = e^{ikx} - e^{-ikx} = 2isin(\pi x/a)$$



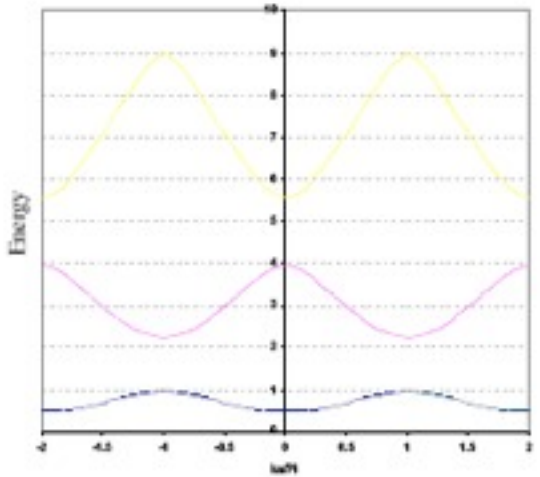
$$U(x) = 2Ucos(2\pi x/a)$$

$$E_g = \int_0 dx\, U(x)\, [\Psi^*_+\Psi_+ - \Psi^*_-\Psi_-] = U$$

Expression of band structure in different schemes



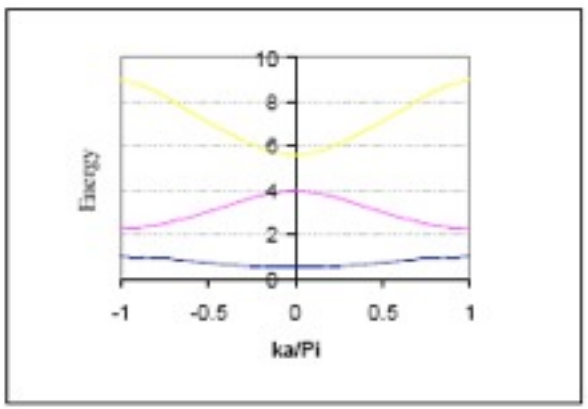
Periodic Zone Scheme



$$\psi_n(\mathbf{k}) = \psi_n(\mathbf{k} + \mathbf{G})$$

$$\epsilon_n(\mathbf{k}) = \epsilon_n(\mathbf{k} + \mathbf{G})$$

Reduced Zone Scheme



•Bands folded into First Brillouin Zone

Tight binding model

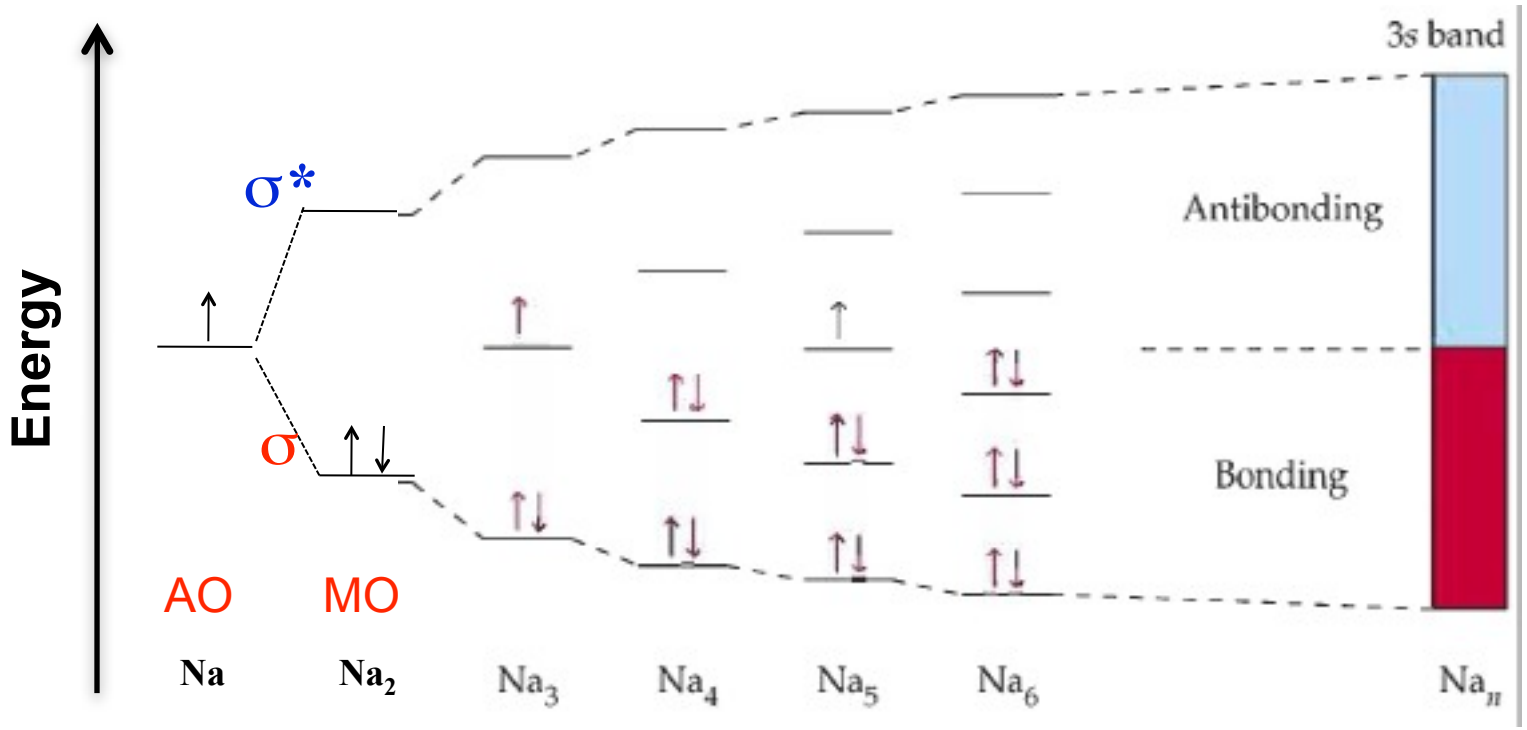
In solid-state physics, the tight binding model is an approach to the calculation of electronic band structure using an approximate set of wave functions based upon superposition of wave functions for isolated atoms located at each atomic site. In this approach, interactions between different atomic sites are considered as perturbations, i.e. correction to the atomic potential ΔU is small.

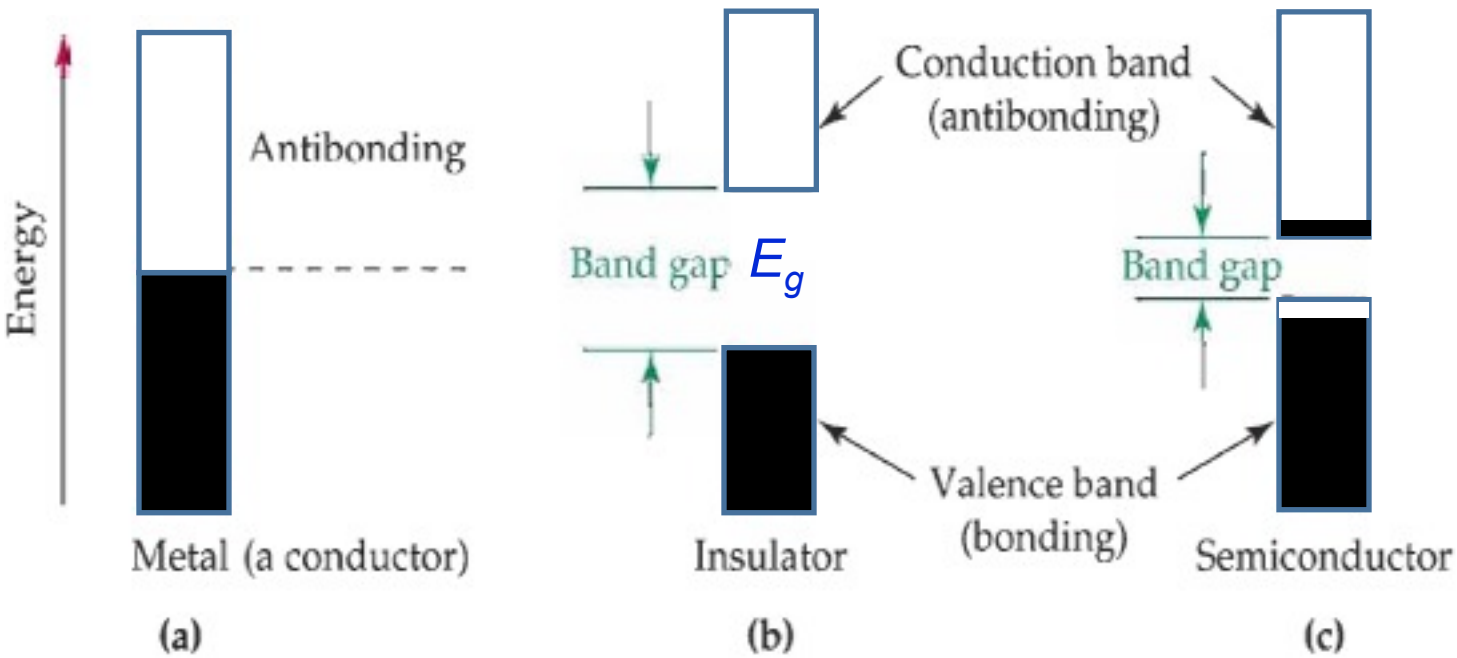
$$H(\boldsymbol{r}) = \sum_{\boldsymbol{R}_n} H_{\mathrm{at}}(\boldsymbol{r} - \boldsymbol{R}_n) + \Delta U(\boldsymbol{r}) \ .$$

A solution ψ(***r***) to the time-independent single electron Schrödinger equation is then approximated as a linear combination of atomic orbitals $\varphi_m(\boldsymbol{r} - \boldsymbol{R}_n)$:

$$\psi(\boldsymbol{r}) = \sum_{m,\boldsymbol{R}_n} b_m(\boldsymbol{R}_n)\ \varphi_m(\boldsymbol{r} - \boldsymbol{R}_n)$$

where *m* refers to the *m-th* atomic energy level and $\boldsymbol{R}_n$ locates an atomic site in the crystal lattice.


Energy
σ*
σ
AO
MO
Na
Na2
Na3
Na4
Na5
Na6
Nan
3s band
Antibonding
Bonding

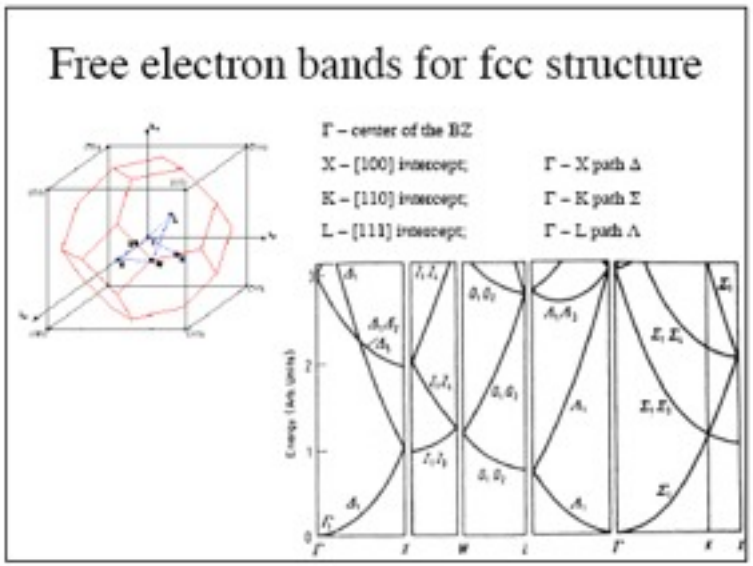


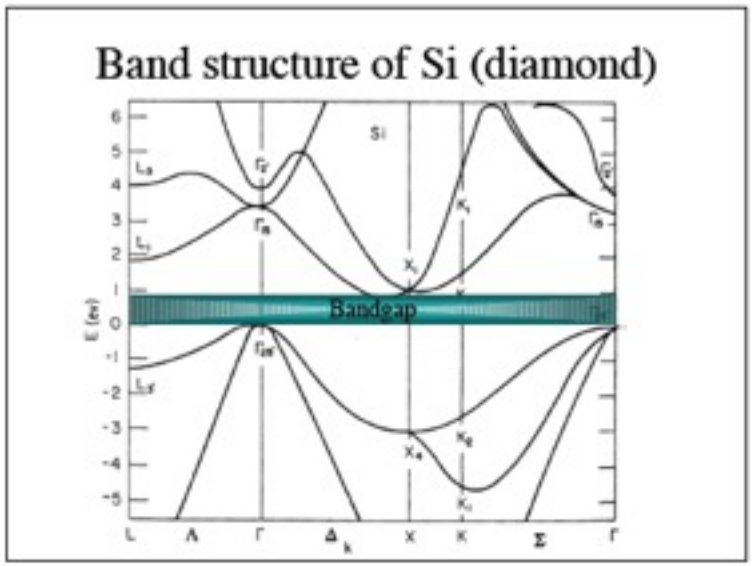
$E_g = 0$

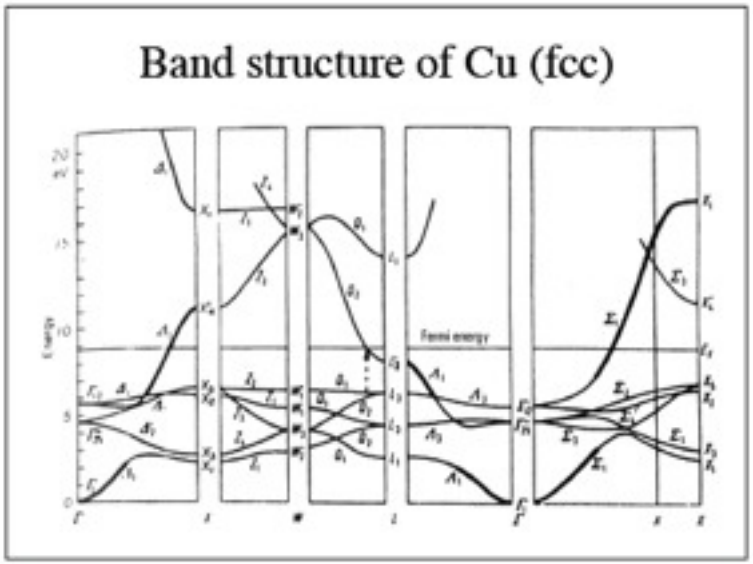
$E_g > 3$ eV

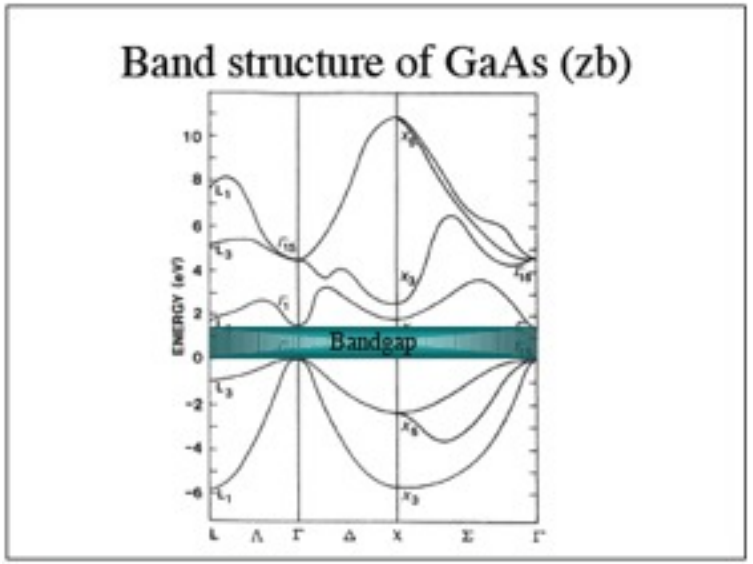
$E_g < 3$ eV

Examples


Free electron bands for fcc structure
Γ – center of the BZ
X – [100] intercept;
K – [110] intercept;
L – [111] intercept;
Γ – X path Δ
Γ – K path Σ
Γ – L path Λ


Band structure of Si (diamond)
Si
Bandgap
E (ev)
L Λ Γ Δ X K Σ Γ


Band structure of Cu (fcc)
Fermi energy

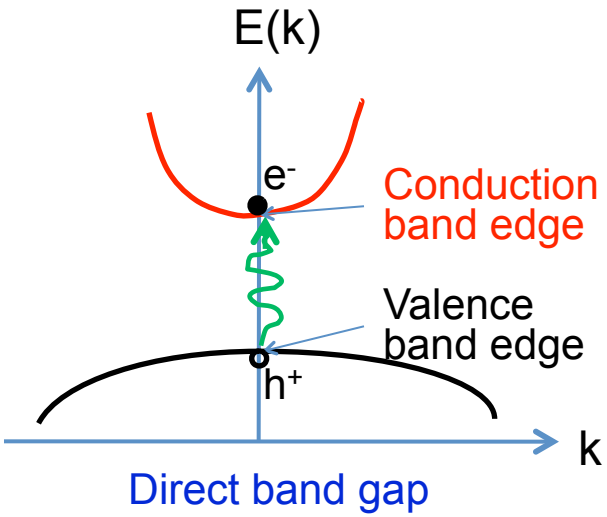

Band structure of GaAs (zb)
ENERGY (eV)
Bandgap
L Λ Γ Δ X Σ Γ

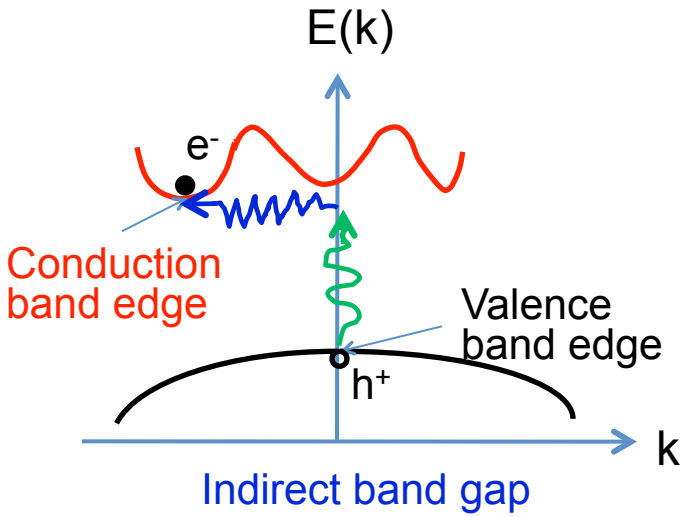
Energy gap between the valence and conduction bands

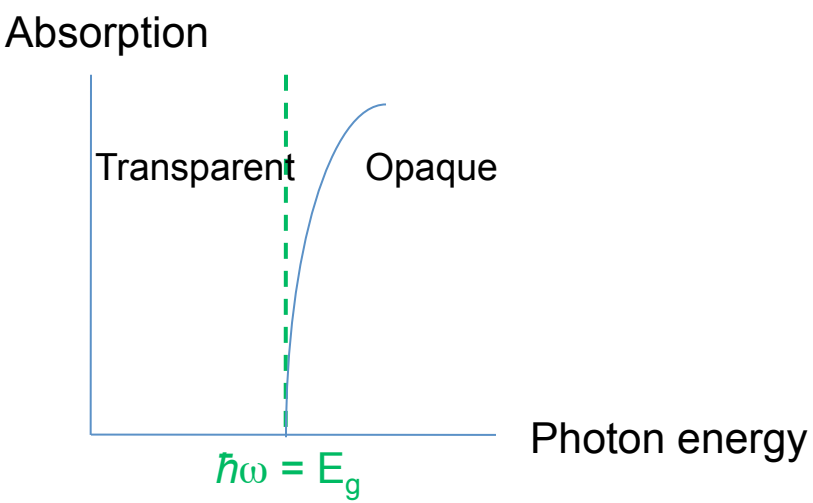
Crystal	Gap	E_g (eV) 0 K	E_g (eV) 300 K	Nomenclature
Diamond	i	5.4		Elemental
Si	i	1.17	1.1	Elemental
Ge	i	0.74	0.66	Elemental
SiC	i	3.0		IV-IV compound
InP	d	1.42	1.27	III-V compound
GaAs	d	1.52	1.43	III-V compound
CdSe	d	1.84	1.74	II-VI compound
ZnO		3.44	3.2	II-VI compound

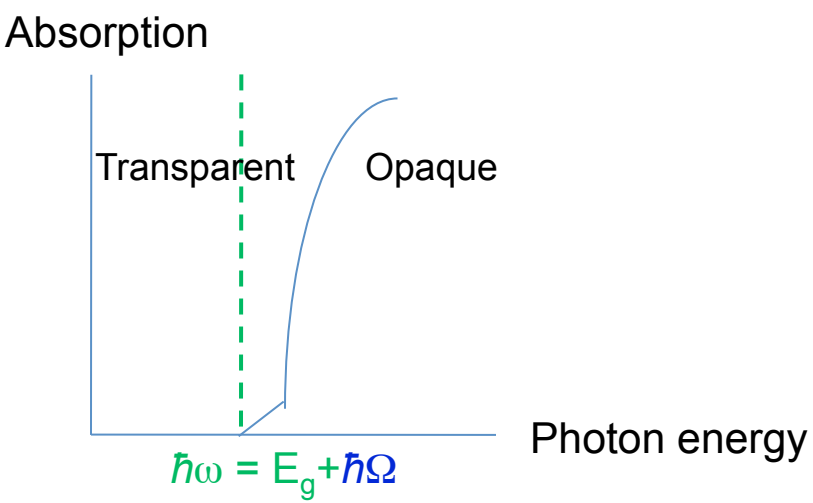
Photo-excitation of semiconductors

One of outstanding characters for semiconductors as a type of materials is their ability to interact with the visible light.

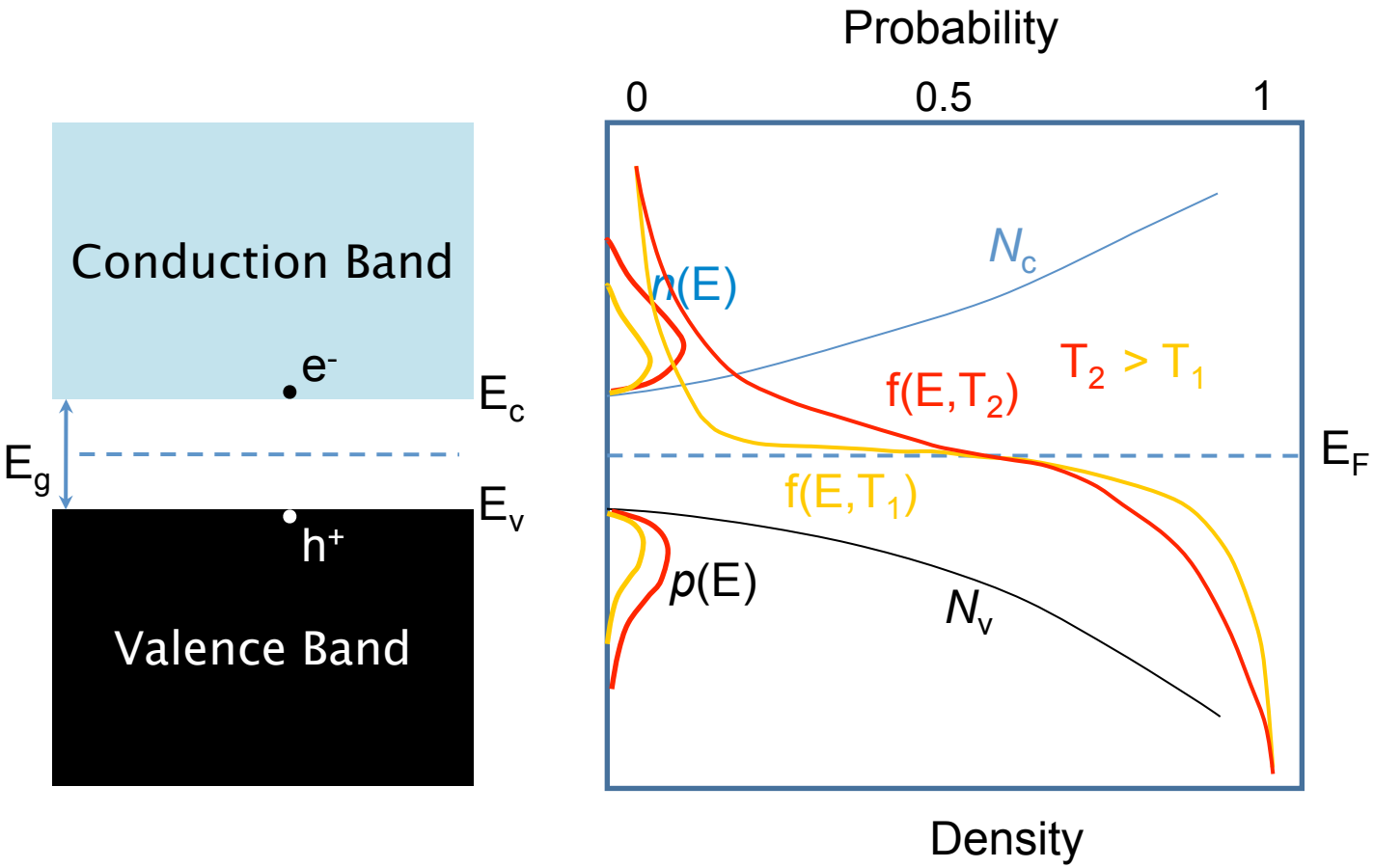








Thermal excitation of semiconductors



$$n(E) = \int_{E_c}^{\infty} N_c(E) f(E)\, dE \qquad p(E) = \int_{-\infty}^{E_v} N_v(E)[1-f(E)]\, dE$$

Intrinsic carriers

The thermal excitation of a carrier from the valence band to the conduction band creates free carriers (electrons and holes) in both bands. The concentration of these carriers is called the intrinsic carrier concentration, denoted by n_i.

$$n_i = \sqrt{N_c N_v}\, e^{-E_g/2kT}$$

where N_c (N_v) is the *effective density of states* in the *conduction (valence) band.*

In an intrinsic semiconductor under thermal equilibrium, the concentration of electrons (n) and holes (p) is equivalent. That is,

$$n = p = n_i$$

For Silicon, $N_c = 2.81 \times 10^{19}$ cm^{-3} and $N_v = 1.83 \times 10^{19}$ cm^{-3}

At T = 300 K (room temperature), $n_i \sim 1.0 \times 10^{10}$ cm^{-3}

Electron and hole

In solid state physics, an **electron hole** (usually referred to simply as a **hole**) is the absence of an electron from the otherwise full valence band. The concept of a hole is essentially a simple way to analyze the electronic transitions within the valence band.

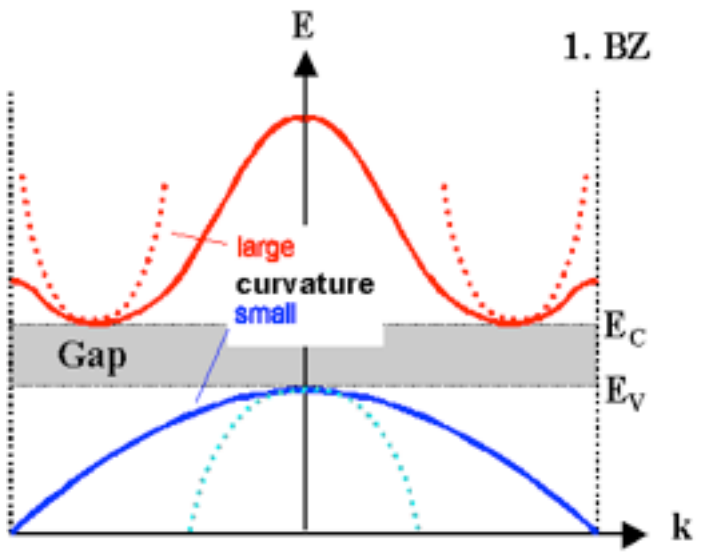
Property	Electron	Hole
Charge	q_e	$q_h = -q_e$
Effective mass	m_e	$m_h = -m_e$
Velocity	$\mathbf{v}_e$	$\mathbf{v}_h = \mathbf{v}_e$
Wavevector	$\mathbf{k}_e$	$\mathbf{k}_h = -\mathbf{k}_e$
Energy	$E_e(\mathbf{k}_e)$	$E_h(\mathbf{k}_h) = -E_e(\mathbf{k}_e)$

Effective mass

A particle's **effective mass (*m**)** is the mass it seems to carry in the *semiclassical model* of transport in a crystal. In a simplified picture that ignores crystal anisotropies, electrons or holes behave as free particles in a vacuum, but with a different mass. This mass is usually stated in units of the ordinary mass of an electron m_e (9.11×10^{-31} kg). In these units it is usually in the range 0.01 or 10.

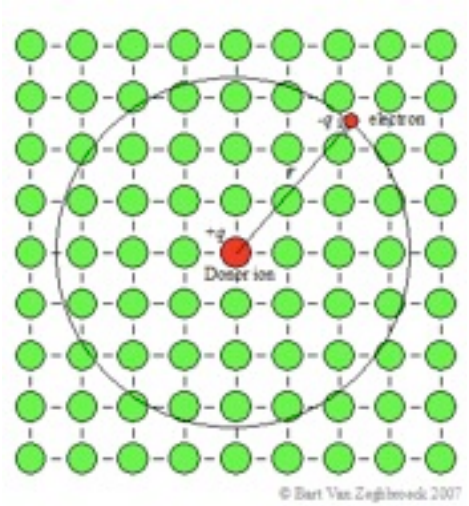
$$m^* = \hbar^2 \cdot \left[\frac{d^2\varepsilon}{dk^2}\right]^{-1}.$$

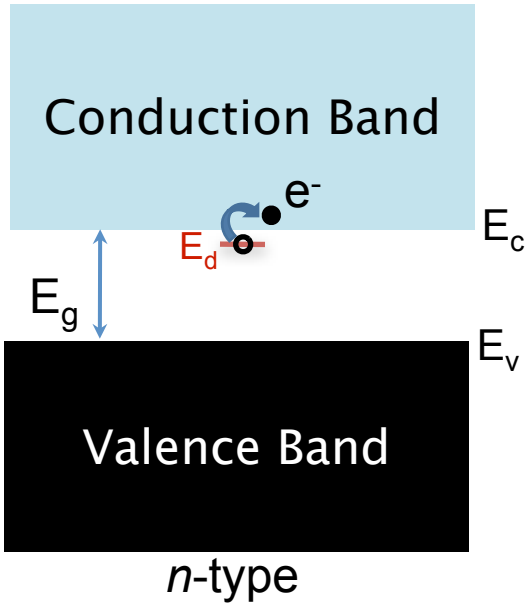
The decisive factor for the effective mass is thus the *curvature of the dispersion curve at the extrema*, as expressed in the second derivative. Large curvatures (*small* radius of curvature) give small effective masses, and vice versa.



Extrinsic semiconductors

Extrinsic semiconductors are semiconductors doped with foreign atoms, which are incorporated into the crystal structure of the semiconductor.





For Hydrogen atom,

$$E_1 = -\frac{e^4}{32\pi^2\hbar^2}\left(\frac{m_e}{\varepsilon_0^2}\right) = -13.6 \text{ eV}$$

For Phosphor-doped n-type

Silicon,

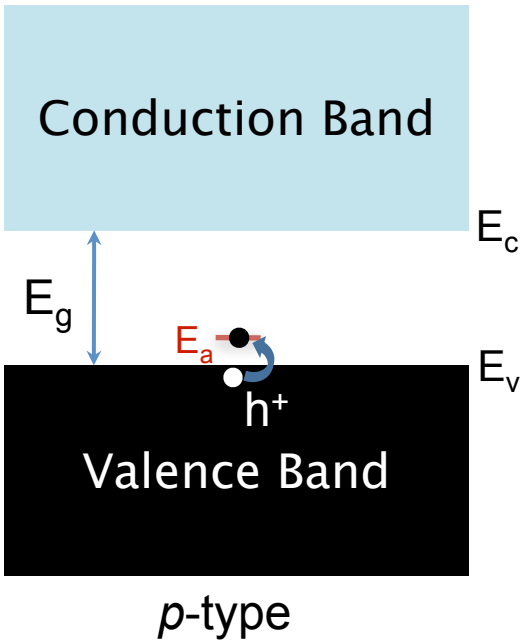
$$E_d - E_c = -13.6 \text{ eV} \times \left(\frac{m^*}{m_e}\right) \times \left(\frac{\varepsilon_0^2}{\varepsilon^2}\right)$$

$m^* = 0.3\, m_e$, $\varepsilon = 12$

$$\rightarrow \quad E_c - E_d \sim 0.03 \text{ eV}$$

$$r = a_0 \times \left(\frac{m_e}{m^*}\right) \times \left(\frac{\varepsilon}{\varepsilon_0}\right) \sim 40\, a_0 \sim 20 \text{ Å}$$

Extrinsic carriers



For *n*-type semiconductors,

$n \sim N_d$, $p \sim p_0$, $n >> p$

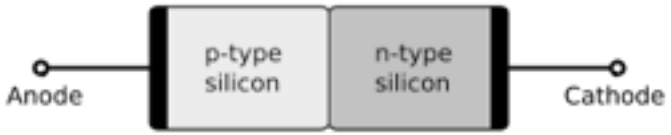
$N_d \equiv$ Concentration of donor dopants

For *p*-type semiconductors,

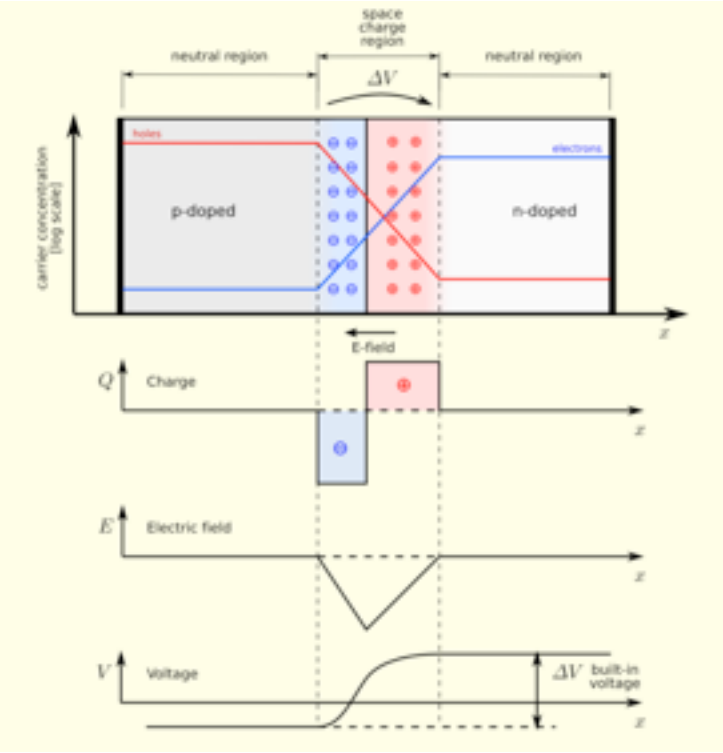
$p \sim N_a$, $n \sim n_0$, $p >> n$

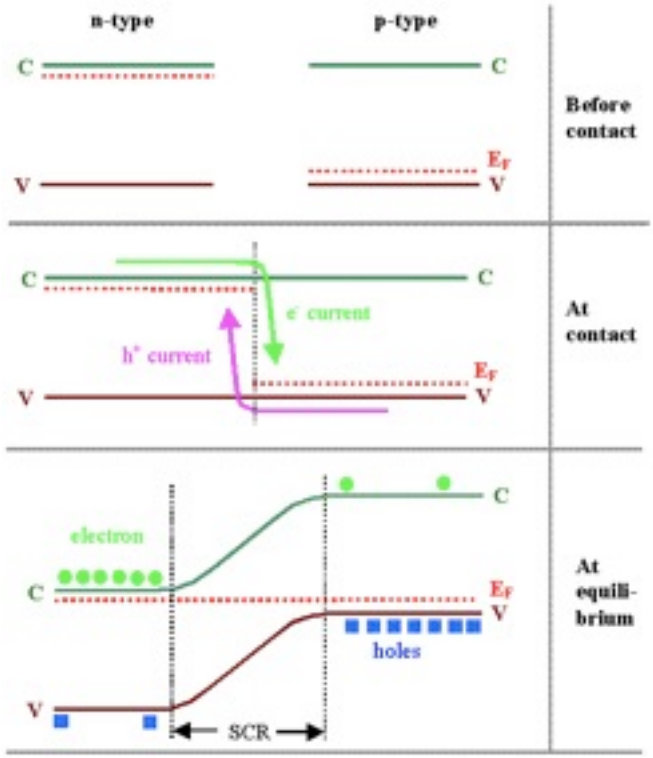
$N_a \equiv$ Concentration of acceptor dopants

p-n junctions



A ***p-n* junction** is a junction formed by joining p-type and n-type semiconductors together in very close contact. The *p-n* junctions are elementary "building blocks" of almost all semiconductor electronic devices such as diodes, transistors, solar cells, LEDs, and integrated circuits; they are the active sites where the electronic action of the device takes place.





Homework#14 (Dec. 20, 2010):

Indium antimonide (InSb) has E_g = 0.23 eV; dielectric constant ε = 18; electron effective mass m* = 0.015 m_e. Calculate (a) the donor ionization energy; (b) the radius of the ground state orbit. (c) At what minimum donor concentration will appreciable overlap effects between the orbits of adjacent impurity atoms occur?


Merry Christmas
Replay
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