Physics of Semiconductor Devices

Lecture 1.

Introduction to the Band Theory of Solids

A.V.Sogoyan

Literature

1. Степаненко И.П. Основы микроэлектроники: Учеб. пособие для вузов. – 2-е изд., перераб. и доп.. – М. : Лаборатория Базовых Знаний, 2001. – 488 с. : ил.
2. *Агаханян, Т.М. Основы транзисторной электроники [Текст] / Т. М. Агаханян. - М. : Энергия, 1974. - 256 с
3. Sah C.-T. Fundamentals of solid-state electronics /C.-T. Sah. World Scientific, 1991. 1011 p.
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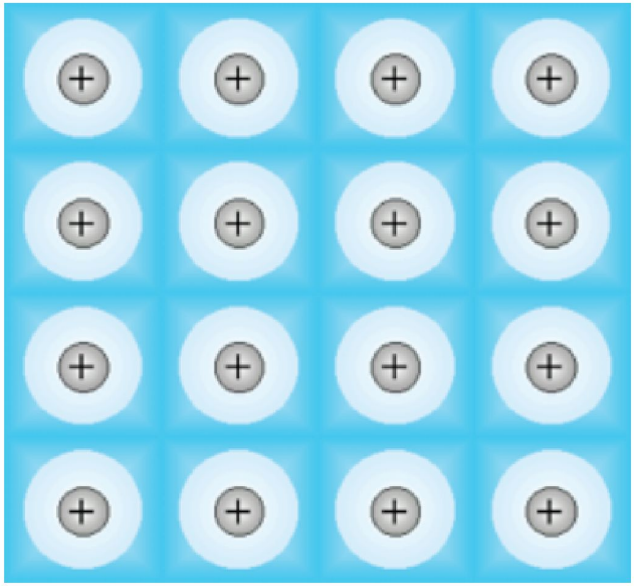
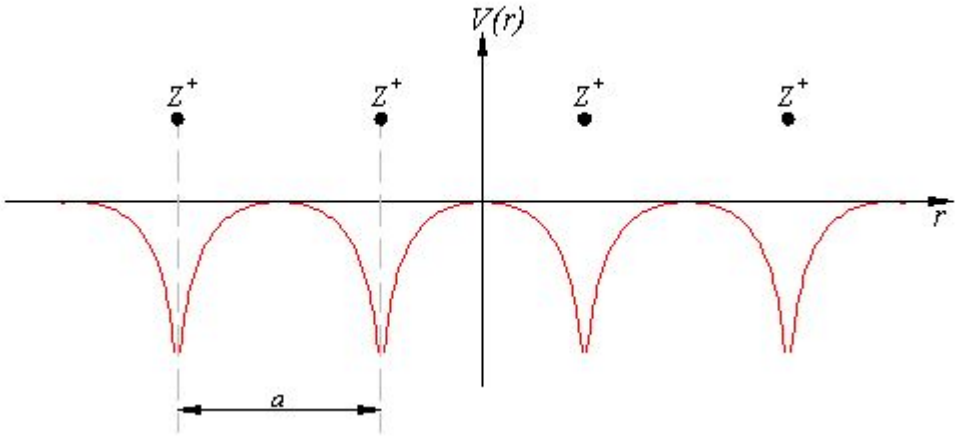
Contents:

- The origin of energy bands in solids. Band diagrams.
- Metals, semiconductors and insulators in the band theory.
- The dependence of the semiconductor bandgap on the temperature.
- The concept of electrons and holes in semiconductors. Effective mass.

The origin of energy bands in solids

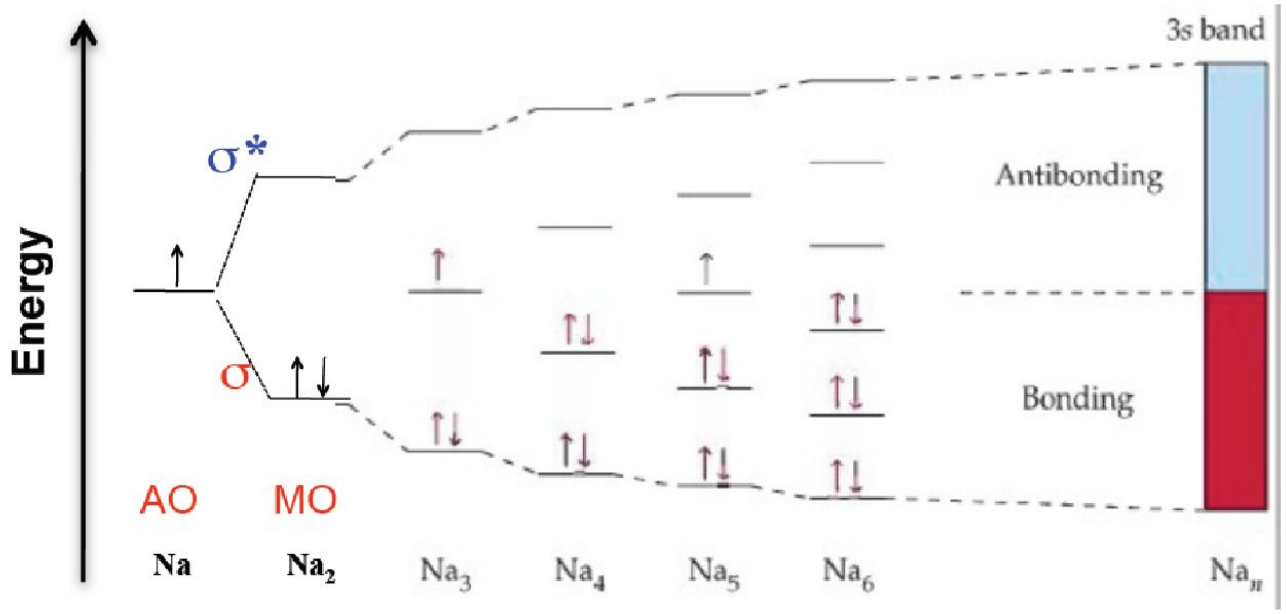




When two single or isolated atoms are bring close to each other then the outermost orbit electrons of two atoms are interact or shared with each other. i.e, the electrons in the outermost orbit of one atom experience a attractive force from the nearest or neighboring atomic nucleus. Due to this the energies of the electrons will not be in same level, the energy levels of electrons are changed to a value which is higher or lower than that of the original energy level of the electron.

The origin of energy bands in solids

The electrons in same orbit exhibits different energy levels. The grouping of this different energy levels is called energy band.



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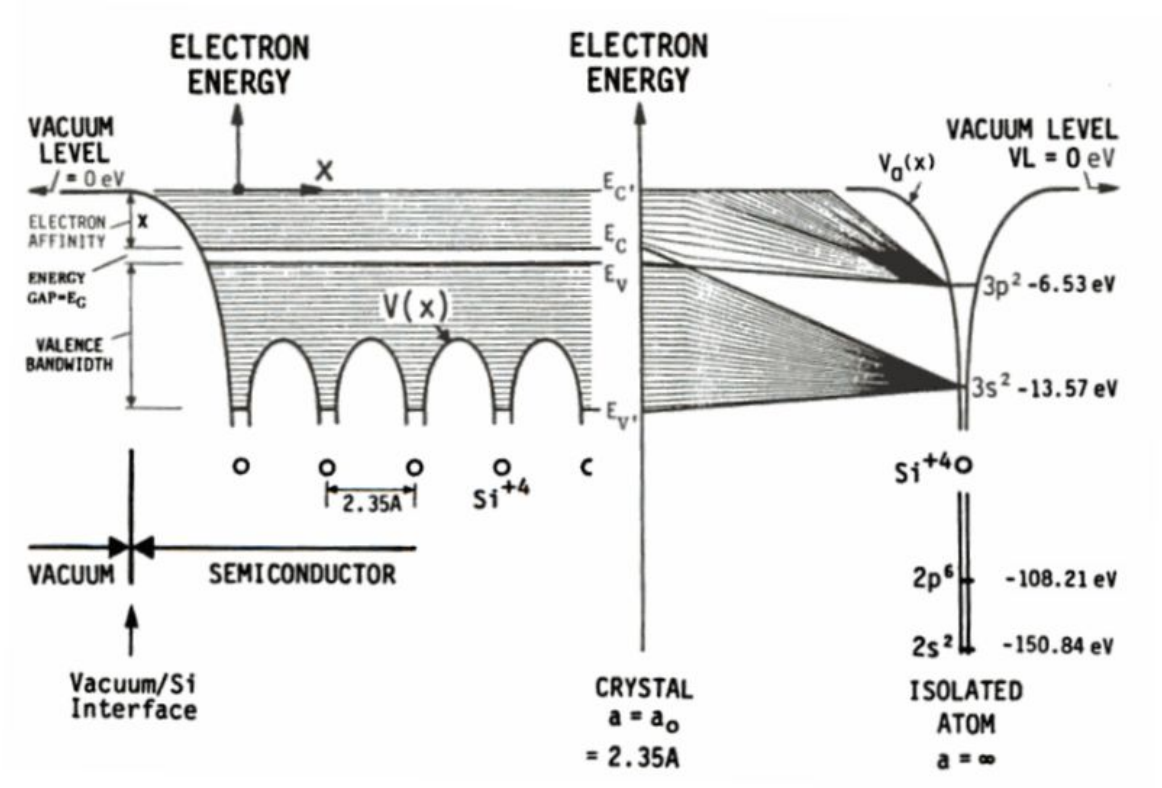
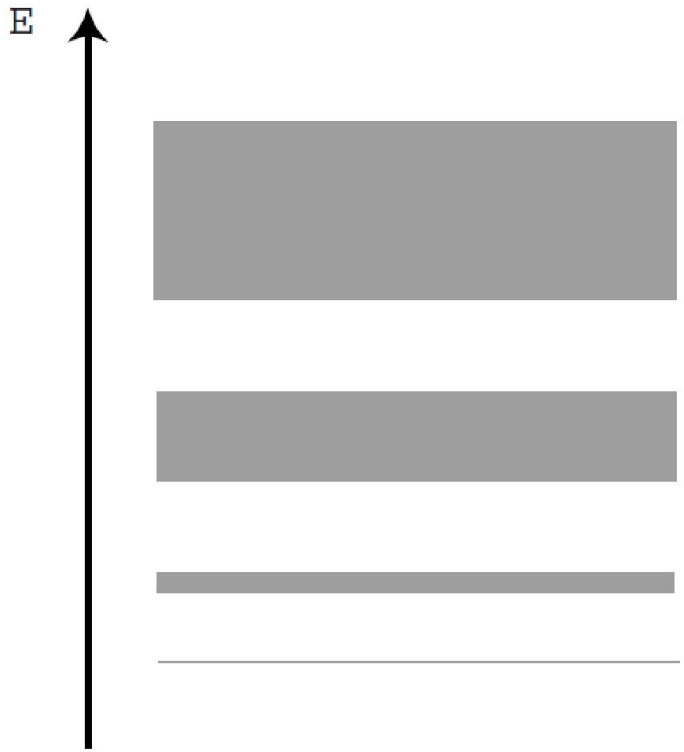
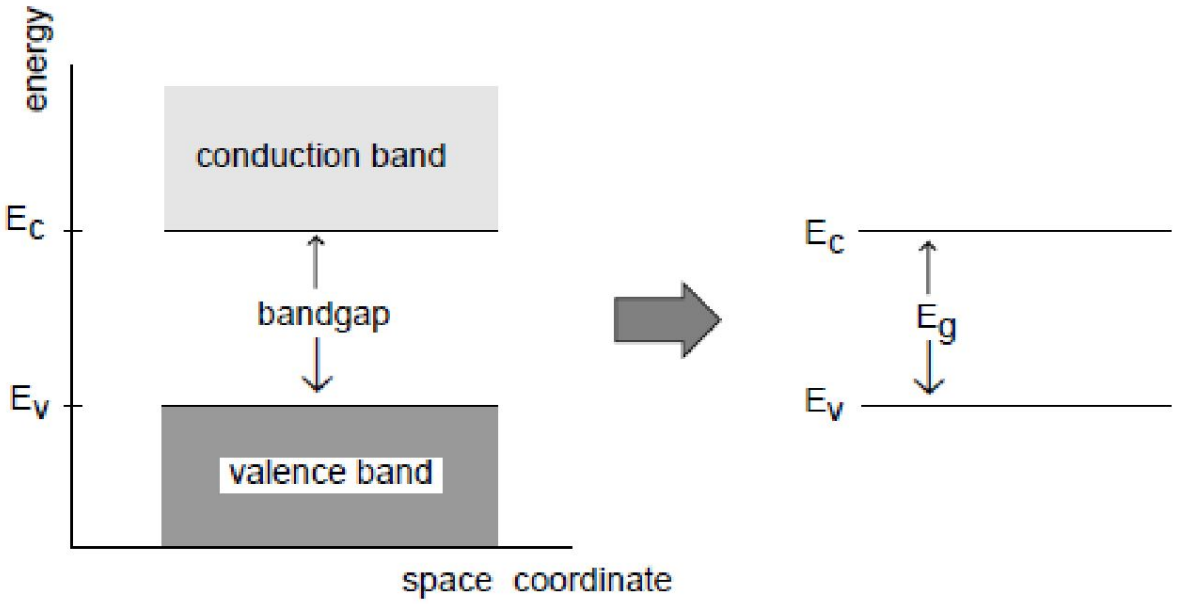


The origin of energy bands in solids

Fundamental result of solid-state physics: *quantum states cluster in bands leaving bandgaps* (regions without allowed states) *in between.*

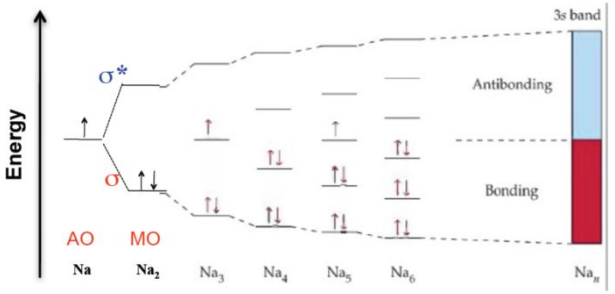


Band diagrams

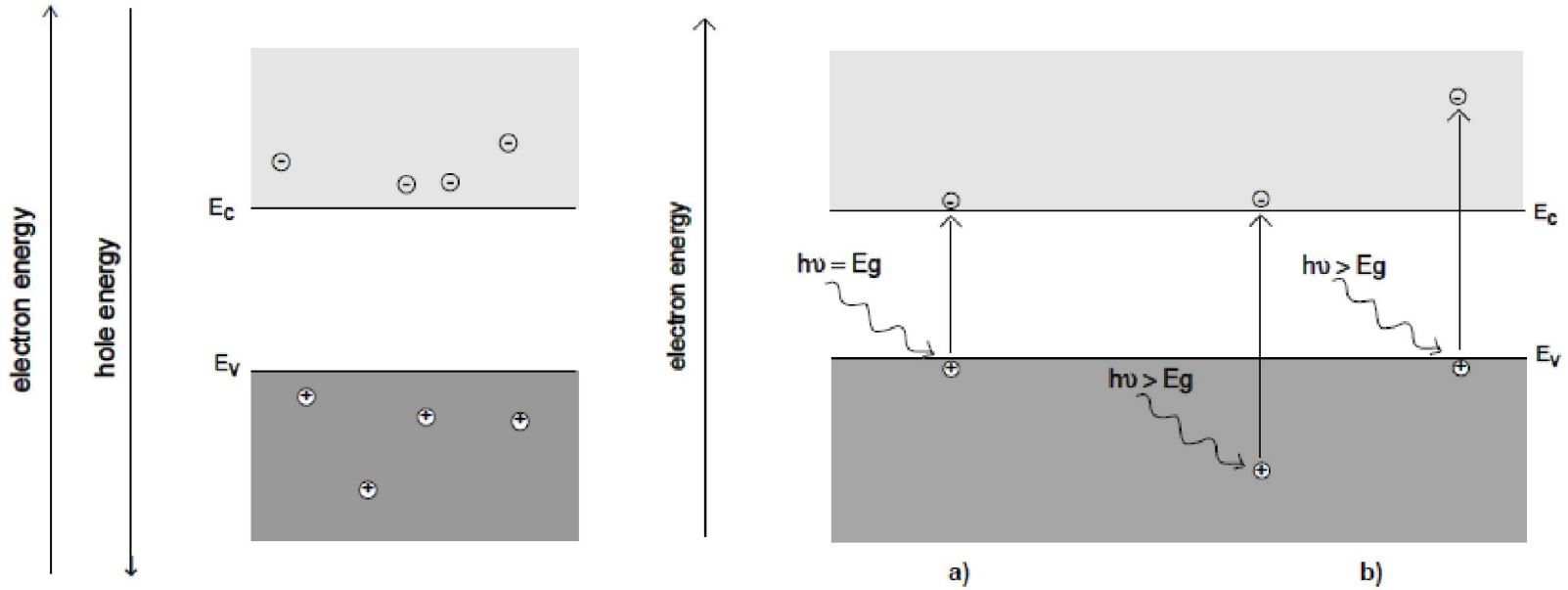


Conduction and valence bands:

- *bonding electrons* occupy states in valence band
- *"free" electrons* occupy states in conduction band
- *holes*: empty states in valence band
- CB electrons and VB holes can move around: *"carriers"*



Band diagrams



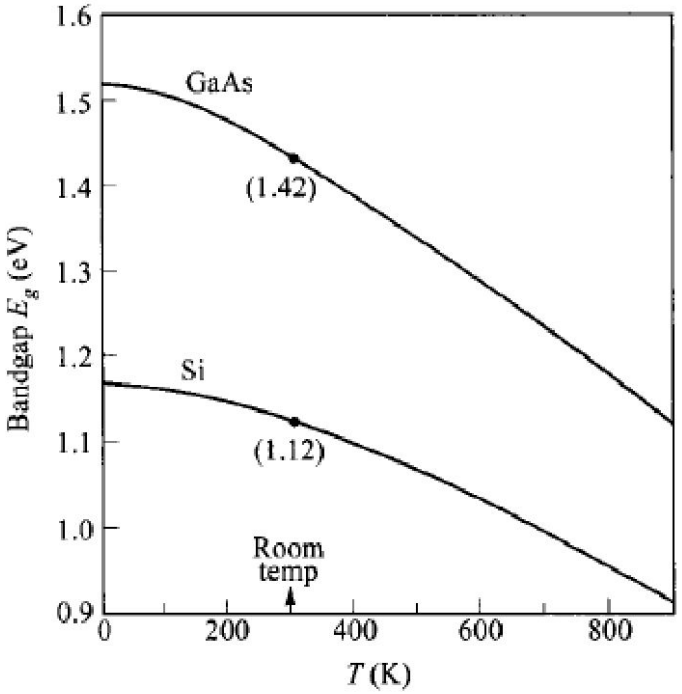
- at edges of bands, kinetic energy of carriers is zero
- electron energies increase upwards
- hole energies increase downwards

The dependence of the semiconductor bandgap on the temperature

At room temperature and under normal atmospheric pressure, the values of the bandgap are 1.12 eV for Si and 1.42 eV for GaAs. These values are for high-purity materials. For highly doped materials the bandgaps become smaller. Experimental results show that the bandgaps of most semiconductors decrease with increasing temperature. Figure 6 shows variations of bandgaps as a function of temperature for Si and GaAs. The bandgap approaches 1.17 and 1.52 eV respectively for these two semiconductors at 0 K. The variation of bandgaps with temperature can be expressed approximately by a universal function

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

The dependence of the semiconductor bandgap on the temperature



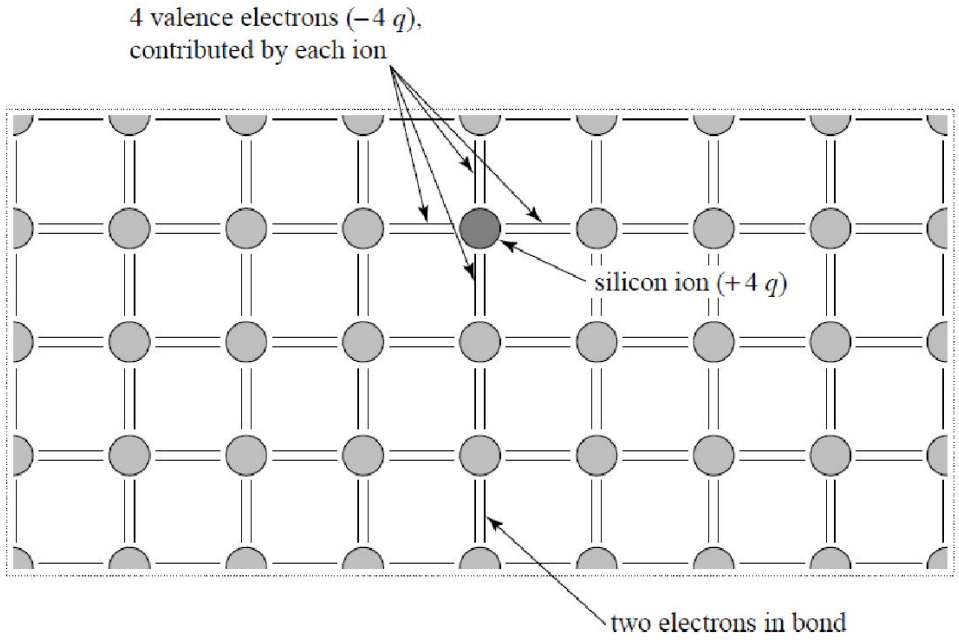
	$E_g(0)$ (eV)	α (eV/K)	β (K)
GaAs	1.519	5.4×10^{-4}	204
Si	1.169	4.9×10^{-4}	655

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

"simplified" form:

$$E_g(T) \approx E_g(T_x) + \frac{dE_g}{dT}\cdot(T - T_x) = E_{g0} - \eta_E T$$

The concept of electrons and holes in semiconductors

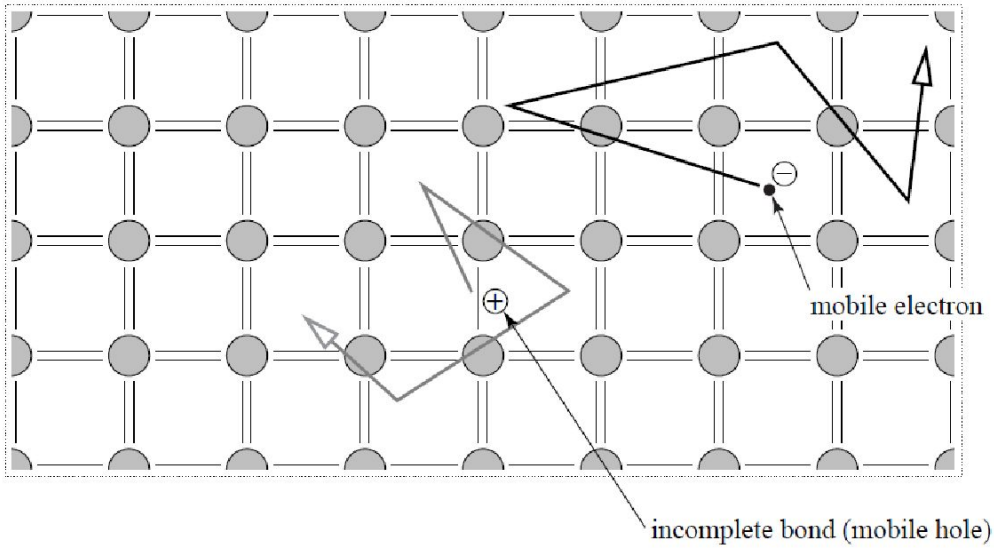


At 0K:

- all bonds satisfied → all valence electrons engaged in bonding
- no "free" electrons

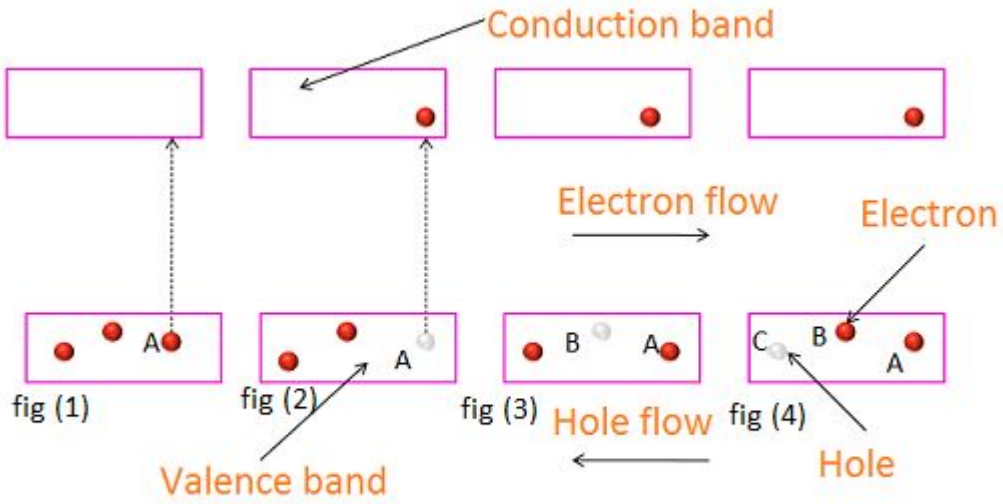
The concept of electrons and holes in semiconductors

At finite temperature:



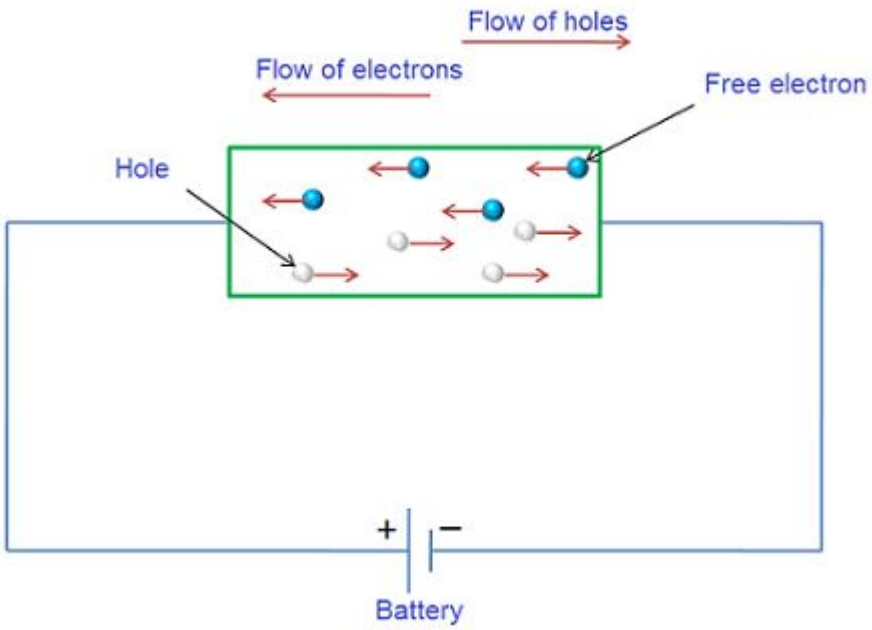
- some bonds are broken
- "free" electrons (mobile negative charge, $-1.6\times10^{-19}\ C$)
- "free" *holes* (mobile positive charge, $1.6\times10^{-19}\ C$)

The concept of electrons and holes in semiconductors



Let's take an example, as shown in fig there are three atoms atom A, atom B and atom C. At room temperature valence electron in an atom A gains enough energy and jumps in to conduction band as show in fig (1). When it jumps in to conduction band a hole (vacancy) is created in the valence band at atom A as shown in fig (2). Then the neighboring electron from atom B moves to atom A to fill the hole at atom A. This creates a hole at atom B as shown in fig (3). Similarly neighboring electron from atom C moves to atom B to fill the hole at atom B. This creates a hole at atom C as shown in fig (4). Likewise electrons moves from left side to right side and holes moves from right

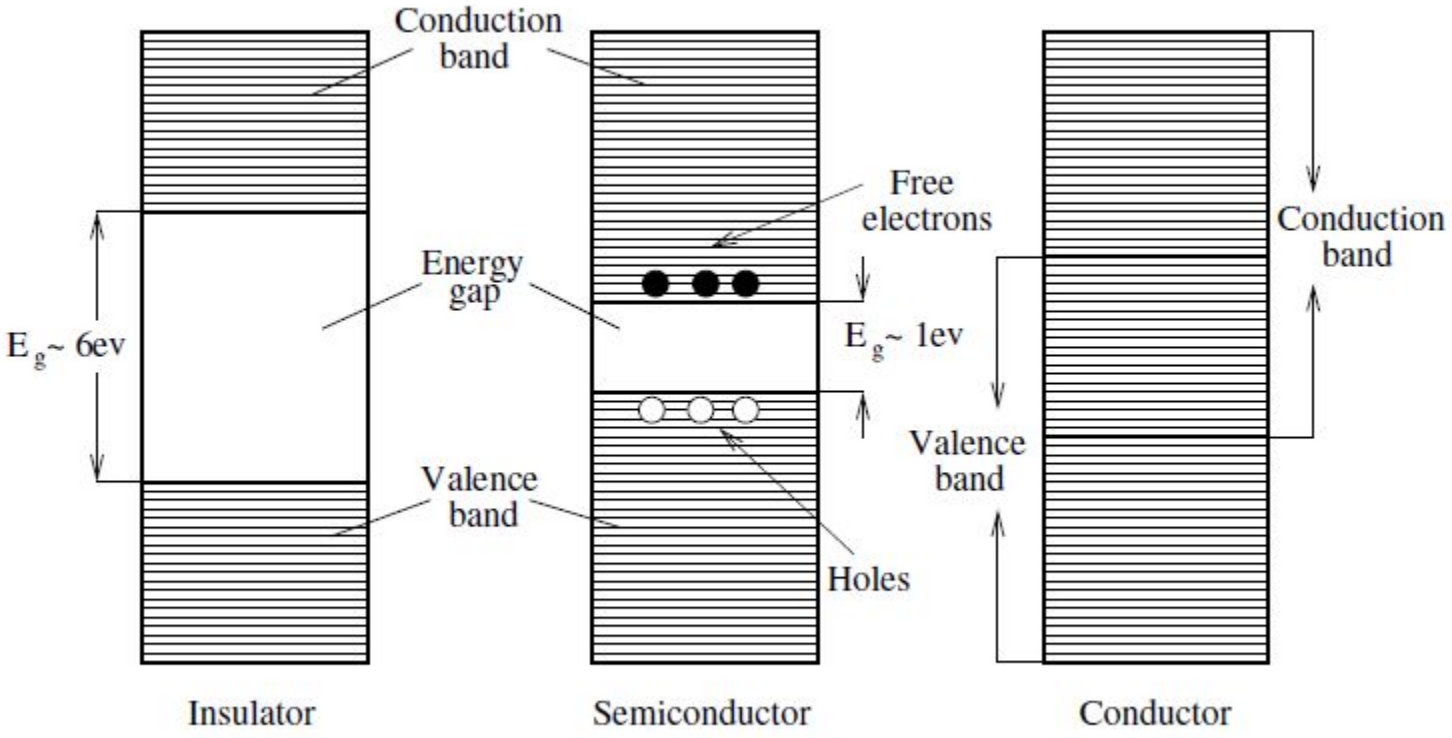
The concept of electrons and holes in semiconductors



The total current in semiconductor is the sum of hole and electron current:

$I = I_{hole} + I_{electron}$

Metals, semiconductors and insulators in the band theory



Energy band structure of conductors, insulators and semiconductors. The valence band is the highest energy band completely filled by electrons at 0K. The conduction band is the next higher possible energy band above the valence band, separated by a forbidden band gap in the case of insulators and semiconductors.

Metals, semiconductors and insulators in the band theory

Distinct feature of semiconductors:

At $0\ K$, filling ends up with full band separated by $1-3\ eV$ bandgap from next empty band.

No conduction is possible in a full band $\Rightarrow$ insulators and semiconductors do not conduct at $0\ K$.

Conduction requires a partially filled band $\Rightarrow$ metals conduct at $0\ K$.

But in semiconductors at finite temperatures, some electrons populate next band above bandgap $\Rightarrow$ conduction becomes possible.

Metals, semiconductors and insulators in the band theory

Electronic structure of Si atom:

- 10 core electrons (tightly bound)
- 4 valence electrons (loosely bound, responsible for most chemical properties)

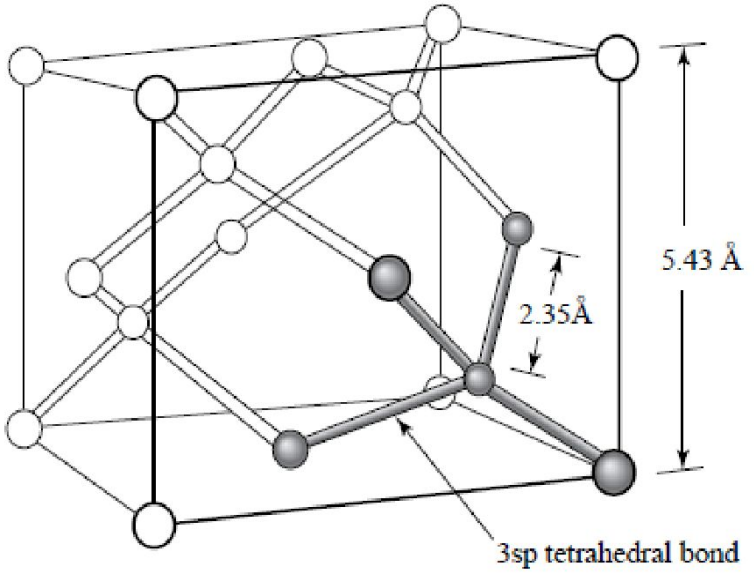
Other semiconductors:

- Ge, C (diamond form), SiGe
- GaAs, InP, InGaAs, InGaAsP, ZnSe, CdTe (on average, 4 valence electrons per atom)

	IIIA	IVA	VA	VIA
	5 B	6 C	7 N	8 O
	13 Al	14 Si	15 P	16 S
IIB				
30 Zn	31 Ga	32 Ge	33 As	34 Se
48 Cd	49 In	50 Sn	51 Sb	52 Te

Metals, semiconductors and insulators in the band theory

- Silicon is a crystalline material:
  - long range atomic arrangement
- *Diamond* lattice:
  - atoms tetrahedrally bonded by sharing valence electrons (*covalent bonding*)
- Each atom shares 8 electrons:
  - low energy and stable situation
- Si atomic density: $5 \times 10^{22}\ cm^{-3}$



Effective mass

Semiclassical Equations of Motion:

$$< \mathbf{v_n(k)} >= \frac{< \mathbf{p} >}{\mathbf{m}} = \frac{\mathbf{1}}{\hbar}\nabla_{\mathbf{k}}\mathbf{E_n(k)}$$

$$\mathbf{F_{ext}} = \hbar\frac{\mathbf{dk}}{\mathbf{dt}}$$

Lets try to put these equations together….

$$a(t) = \frac{dv}{dt} = \frac{1}{\hbar}\frac{\partial}{\partial t}\frac{\partial E_N(k)}{\partial k} = \frac{1}{\hbar}\frac{\partial^2 E_N(k)}{\partial k^2}\frac{dk}{dt}$$

$$= \left[\frac{1}{\hbar^2}\frac{\partial^2 E_N(k)}{\partial k^2}\right] F_{\text{ext}}$$

Looks like Newton's Law if we define the mass as follows…

$$m^*(k) = \hbar^2\left(\frac{\partial^2 E_N(k)}{\partial k^2}\right)^{-1}$$

dynamical effective mass

→ mass changes with k…so it changes with time according to k

Effective mass

Extension to 3-D requires some care,

F and a don't necessarily point in the same direction

$$\mathbf{a} = \overline{\overline{\mathbf{M}}}^{-1}\mathbf{F}_{\text{ext}} \quad \text{where} \quad \overline{\overline{\mathbf{M}}}^{-1}_{i;j} = \frac{1}{\hbar^2}\frac{\partial^2 E_N}{\partial k_i \partial k_j}$$

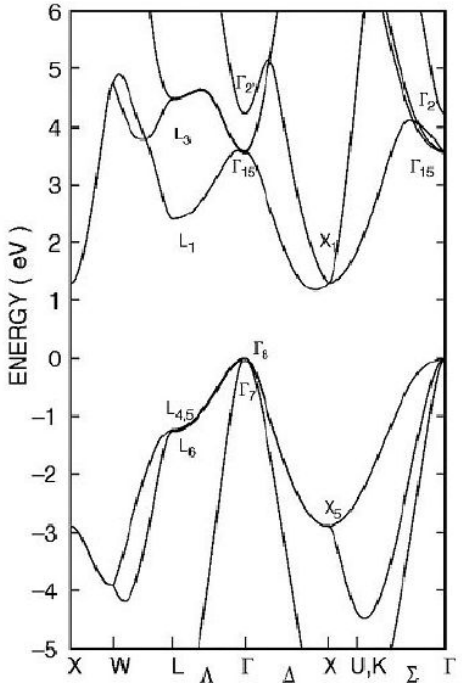
$$\begin{pmatrix} a_x \\ a_y \\ a_z \end{pmatrix} = \frac{d}{dt}\begin{pmatrix} v_x \\ v_y \\ v_z \end{pmatrix} = \begin{pmatrix} \frac{1}{m_{xx}} & \frac{1}{m_{xy}} & \frac{1}{m_{xz}} \\ \frac{1}{m_{yx}} & \frac{1}{m_{yy}} & \frac{1}{m_{yz}} \\ \frac{1}{m_{zx}} & \frac{1}{m_{zy}} & \frac{1}{m_{zz}} \end{pmatrix}\begin{pmatrix} F_x \\ F_y \\ F_z \end{pmatrix}$$

Effective mass

Ellipsoidal Energy Surfaces

Fortunately, energy surfaces can often be approximate as…

$$E_N(k) = E_c + \frac{\hbar^2}{2}\left(\frac{(k_x - k_x^0)^2}{m_t} + \frac{(k_y - k_y^0)^2}{m_t} + \frac{(k_z - k_z^0)^2}{m_l}\right)$$



$$\overline{\overline{\mathbf{M}}}^{-1} = \begin{pmatrix} \frac{1}{m_t} & 0 & 0 \\ 0 & \frac{1}{m_t} & 0 \\ 0 & 0 & \frac{1}{m_l} \end{pmatrix}$$

$$\overline{\overline{\mathbf{M}}} = \begin{pmatrix} m_t & 0 & 0 \\ 0 & m_t & 0 \\ 0 & 0 & m_l \end{pmatrix}$$

Conclusions

1. The energy spectrum of an electron in a crystal is a set of allowed energy bands, separated by forbidden energy bands. The energy spectrum of the allowed bands in most cases can be regarded as quasi-continuous.
2. The formation of bands is due to the overlap of the wave functions of the electrons of the atoms TT.
3. An electron in a crystal in electromagnetic processes behaves as a particle with a certain effective mass m, that differs from the mass of a free particle. Due to the wave properties of the electron effective mass can be either positive or negative and will depend on the direction of motion of an electron in a crystal.
4. E vacancy in the valence band is called a hole. The hole is a quasi-particle; its properties are determined by the collective behavior of the other electrons fill the area.
5. The holes are attributed to the positive charge and effective mass