

Part 2: Semiconductor Basics

Structure, energy bands, doping (résumé)

Electronic conduction in semiconductors

Silicon and III-V materials

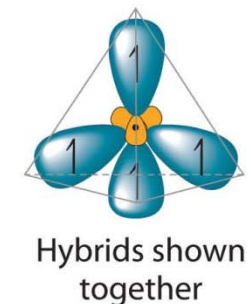
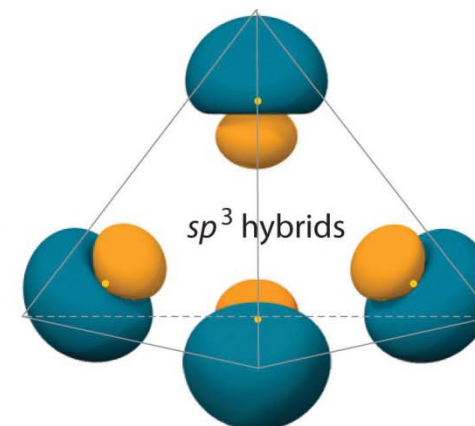
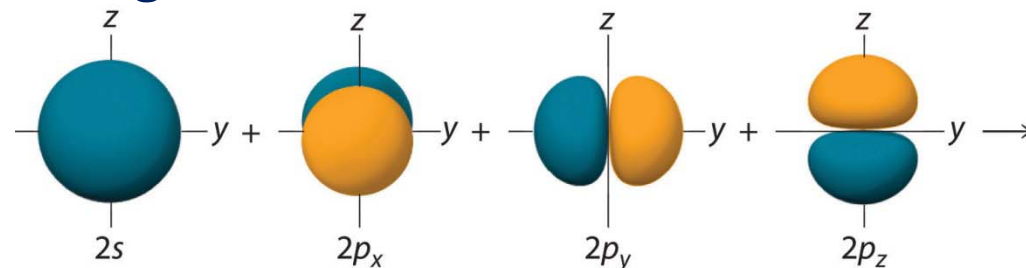
Heterojunctions

Semiconductor bonding and structure

Semiconductors such as silicon are in the middle of the periodic table, with 4 electrons in their outer shell. It needs an extra 4 p-electrons to complete its atomic shell. This can be done by bonding and sharing electrons with 4 adjacent Si atoms

Group III	Group IV	Group V
B $2s^2, 2p^1$	C $2s^2, 2p^2$	N $2s^2, 2p^3$
Al $3s^2, 3p^1$	Si $3s^2, 3p^2$	P $3s^2, 3p^3$
Ga $4s^2, 4p^1$	Ge $4s^2, 4p^2$	As $4s^2, 4p^3$
In $5s^2, 5p^1$	Sn $5s^2, 5p^2$	Sb $5s^2, 5p^3$

To do this, the orbital's must undergo sp^3 hybridisation to produce 4 identical bonds which are configured in a tetrahedron



Semiconductor bonding and structure

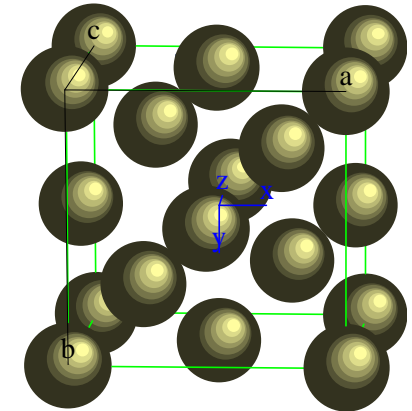
The sp^3 bonds have mixed 's-like' and 'p-like' character - origin of the energy bands in the semiconductor

The tetrahedral bonding to adjacent atoms is replicated in the formation of large crystal structures

The high-symmetry of crystal structures gives rise to strong electronic conduction, but only for certain wavevectors

The inclusion of other elements with different covalency can give rise to doping effects.

P is a common n-type dopant in silicon and has one additional electron. Bonded in a Si lattice it will readily give up this electron, which will then be only very loosely bound to its host. Conversely, Ga is a p-type dopant in Si, which will take electrons from the host crystal creating a hole.

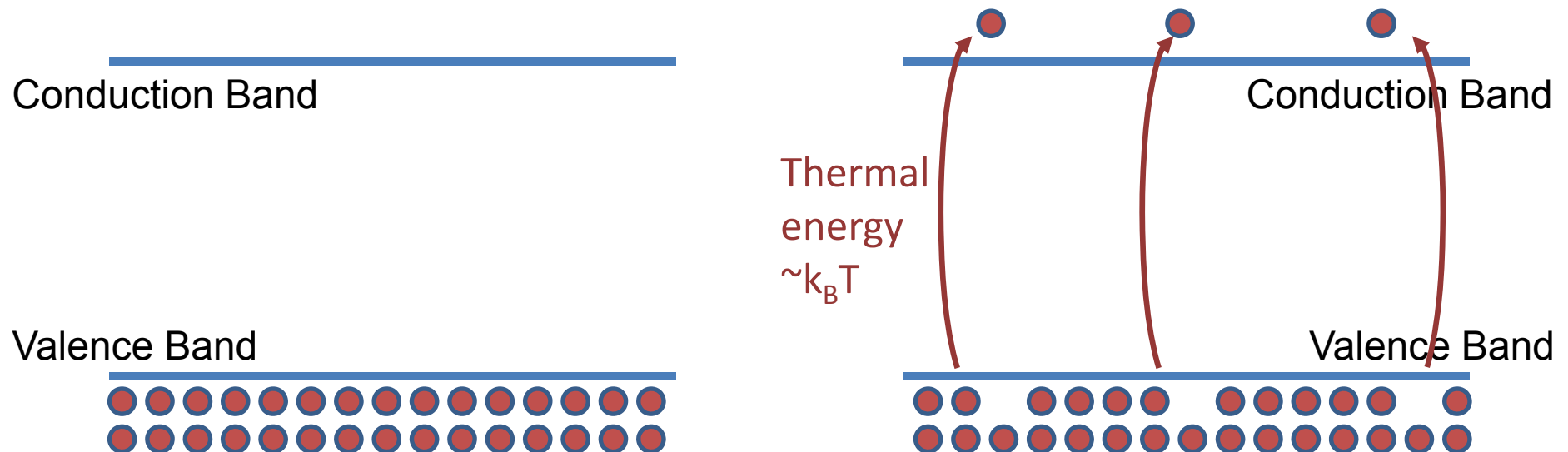


Energy Bands

Semiconductors are characterised by a energy gap ($\sim 1\text{eV}$) which separates a band of filled states (valence band) from a band of empty states (conduction band).

Conduction cannot occur in filled bands, so at low temperatures no conduction occurs

At higher temperatures a finite number of electronics may gain sufficient thermal energy to reach the conduction band



Electronic conduction in semiconductors

Conduction can now occur through the following processes

- **Electrons moving in to empty states in the conduction band**
- **Electrons moving into vacated states in the valence band.**

It is much easier to think of this as the movement or conduction of **'holes' in the valence band**. The hole moves in the opposite direction.

At room temperature silicon has an intrinsic carrier concentration of $1.5 \times 10^{10} \text{cm}^{-3}$. This is a small number compared to the density of silicon atoms ($5 \times 10^{22} \text{cm}^{-3}$) and as a result the conduction is very weak.

Fortunately most semiconductors can be doped to change their conductivity. Typical doping levels can reach $5 \times 10^{19} \text{cm}^{-3}$ (0.1%) or higher before solubility problems set in.

Electronic conduction in semiconductors

Carrier velocity and current density

Carrier velocity $v = \mu E$ ($\mu = \text{mobility}$, $E = \text{electric field}$)

The mobility, μ , is material dependent. It is related to the carrier lifetime (between scattering events) and the carrier mass

$$\mu = \frac{e\tau}{m}$$

Large variations in mobility exist between materials. There is a general trend of higher mobility for smaller band gap. Note also that holes tend to have much lower mobility than electrons

Semiconductor	Si (silicon)	Ge (germanium)	GaAs (gallium arsenide)	InP (indium phosphide)	InAs (indium arsenide)
$\mu_h (\text{holes}) \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$	450	1900	400	150	460
$\mu_e (\text{electrons}) \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$	1500	3900	8500	4600	33000

Electronic conduction in semiconductors

The mass, m , is normally represented by a factor m^* which multiplies the free electron mass m_0 ($m = m^* m_0$)

The mass can represent both electrons and holes, which may have very different values. It is also highly material dependent.

For Si the electron effective mass is 0.19 and the holes 0.49.

Holes are typically much heavier than electrons. This is because they are moving in a band which is almost full of electrons

Note: effective masses of < 1 imply that carriers behave as if they have a smaller mass than a free electron. They are more easily accelerated through the periodic potential of the crystal than they would be in vacuum

Electronic conduction in semiconductors

Effective mass characterised by the dispersion (E versus k relationship). k is proportional to the particle momentum

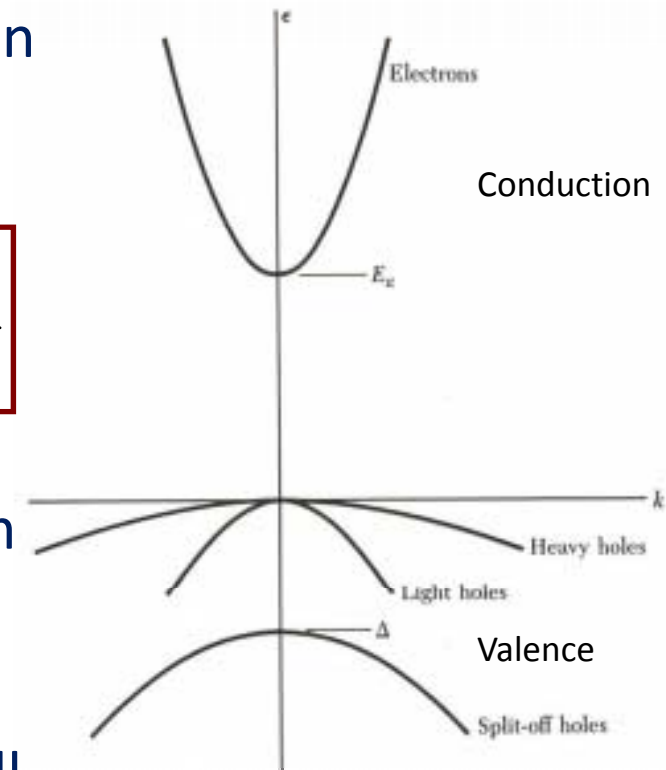
Effective mass is proportional to the radius of curvature

$$E_k = \frac{\hbar^2 k^2}{2m}$$

Conduction band- radius of curvature small, effective mass small. A change in momentum will result in a large change in energy

Valence band- large radius of curvature. A large change in momentum gives only a small change in energy.

Note several Valence bands. We would normally only consider the heavy and light hole bands (heavy holes dominate)



Electronic conduction in semiconductors

Carrier lifetime, τ

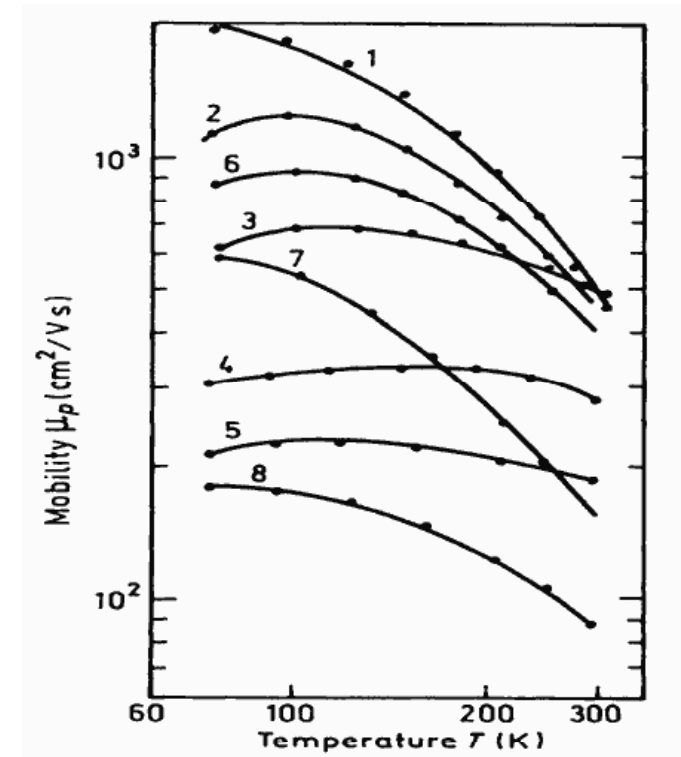
This is related to the number of scattering events, which impede the flow of carriers. There are a few possible processes.

Ionised impurities- **Important for highly doped semiconductors**

Phonons (lattice vibrations)- **Dominant at high temperatures**

Alloy fluctuations (random composition fluctuations in alloys)- **Issue for alloy semiconductors such as SiGe, InGaAs**

Defects (imperfections in crystal lattice) – **Need low defect density materials**



Mobility versus temperature for GaAs with different doping levels

Electronic conduction in semiconductors

Current density (J)

$$J = ne v = \frac{ne^2 \tau}{m^*} E$$

Related to the number of carriers (n) and their velocity (v)

High velocity \rightarrow high current

\rightarrow reduced transit time through the device

\rightarrow reduced capacitance charging time

Prefer

- 1) Highly doped transit regions
- 2) Low effective mass (m^*) materials
- 3) Long scattering lifetimes (τ)

But 1) is somewhat at odds with 3). High doping gives rise to high ionised impurity scattering

Electronic conduction in semiconductors

High field Transport

The previous description is only good for the low E-field case

It implies that in perfect crystals at low temperatures (no scattering losses) that the electron (or hole) would continue to accelerate in an electric field according to their effective mass.

In real crystals electrons (and holes) exhibit velocity saturation at high fields.

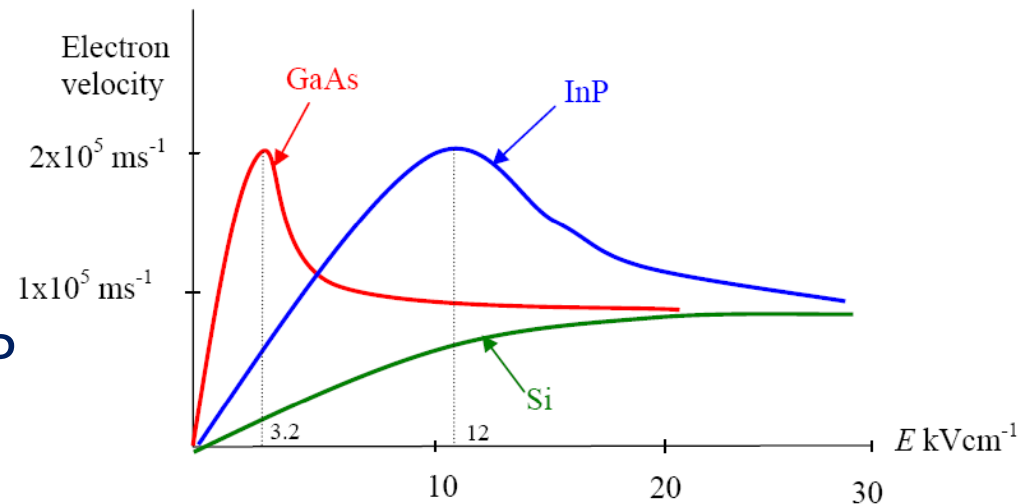
As electrons (and holes) accelerate, they climb further (drop further) in their bands. Here they begin to interact (scatter) with other bands.

The result of this is that most semiconductors exhibit a pronounced velocity saturation. At certain fields, the carrier velocity saturates and may even begin to fall.

Electronic conduction in semiconductors

For silicon, this occurs at an E-field of about 20 kV.cm^{-1} . The velocity reaches $1 \times 10^5 \text{ m.sec}^{-1}$ and never exceed this.

Materials such as GaAs and InP have a higher saturation velocity. However they suffer from a drop in velocity at high fields



Why is this important?

As devices become smaller & smaller to improve speed, some very high electric fields can be encountered.

Electronic conduction in semiconductors

Typical CMOS FET: $E = \frac{V}{d} = \frac{1V}{50nm} = 2 \times 10^5 V.cm^{-1} = 200kV.cm^{-1}$

This is well into the saturation regime. A (low field) mobility calculation would significantly overestimate the speed

Empirical form of the velocity saturation as a function of the electric field E
($E_c = 7 kV/cm^{-1}$ and $v_0 \cong 1 \times 10^5 ms^{-1}$)

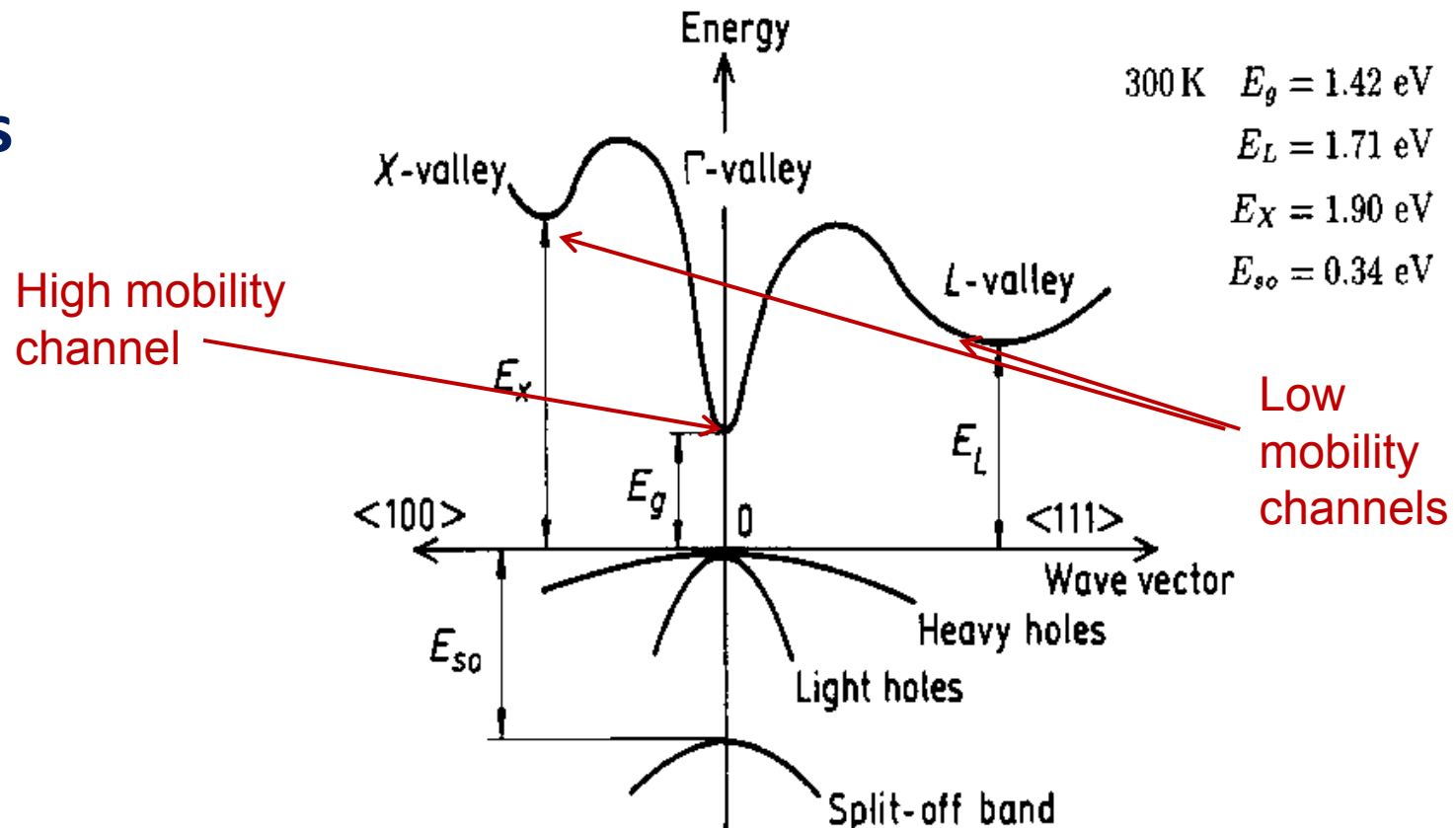
$$V = V_0 \left(\frac{\frac{E}{E_c}}{1 + \frac{E}{E_c}} \right)$$

Why does the velocity decrease at high field for semiconductors such as GaAs and InP?

Electronic conduction in semiconductors

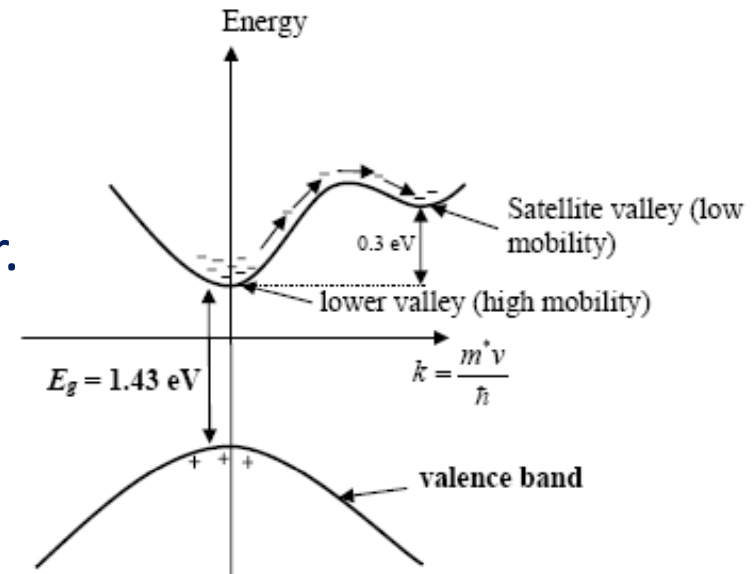
Many compound semiconductors, such as GaAs and InP, have a higher saturation velocity than Si, but suffer from lower mobility higher order channels (satellites)

GaAs

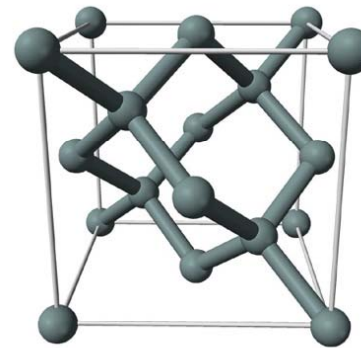


Electronic conduction in semiconductors

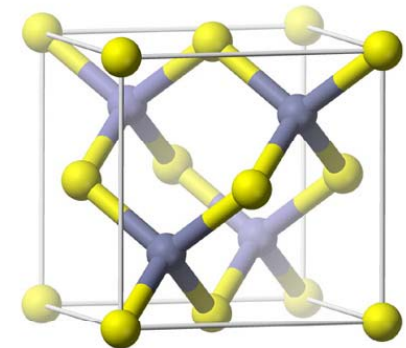
At high electric fields the electrons have enough energy to transfer to a satellite valley where the effective mass is higher. This results in an overall lowering of the velocity as the field increases as more electrons transfer.



Compound semiconductors such as GaAs and InP are made up of two or more elements of different electronegativity.. Gives strong directional mobility and scattering effects



Si

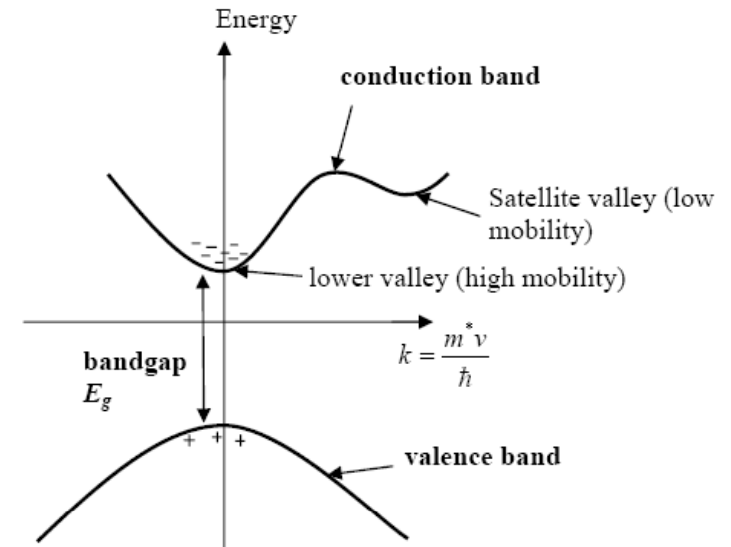
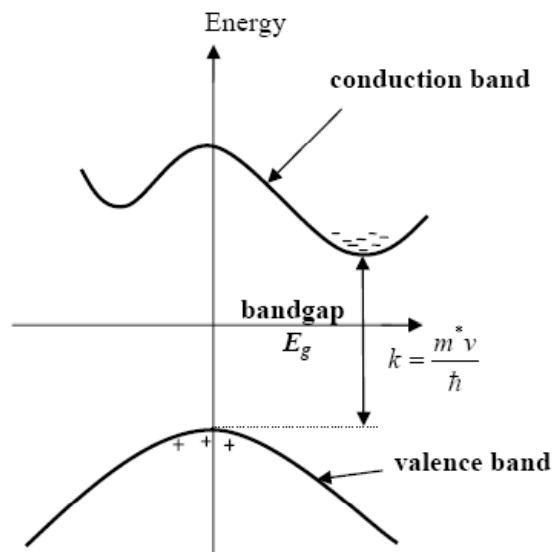


GaAs

Types of band structure

Direct Gap example (=GaAs)

Conduction band minimum is coincident in k-space with hole maximum (both $k=0$)

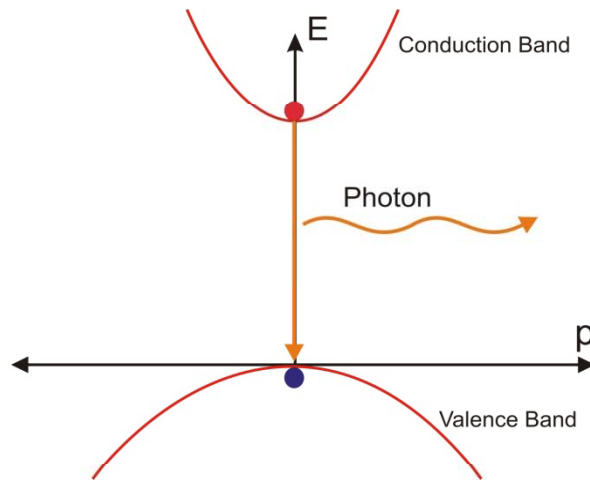


Indirect Gap example (=Si)

Electron energy minimum is not coincident in k-space with hole maximum

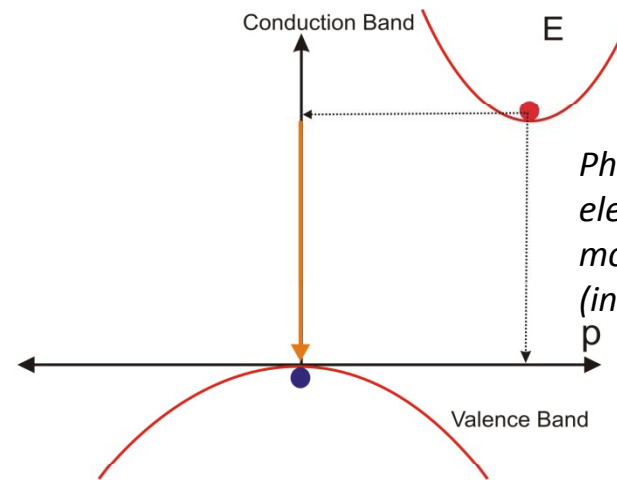
- Photons (light) have a lot of energy, but little momentum.
- Phonons (lattice vibrations) have low energy but high momentum

Types of band structure



Direct Gap

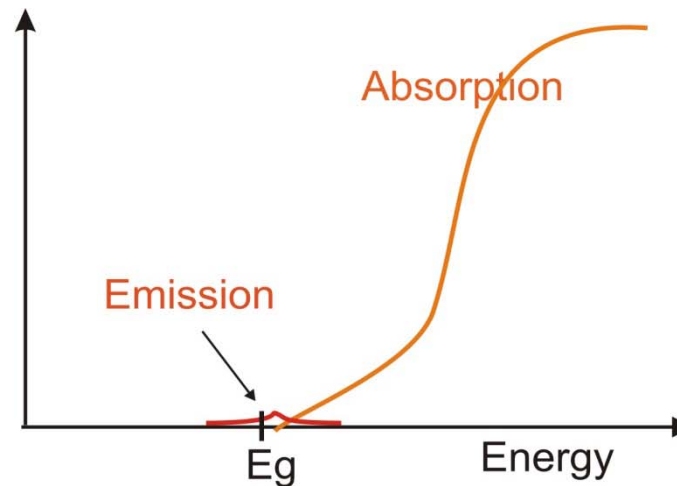
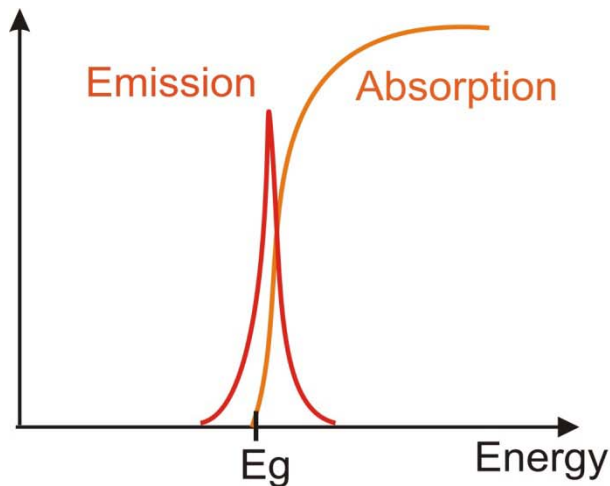
Efficient light emitter. E.g: GaAs, InP, InAs, GaN etc



Photon has little momentum, so electron needs to lose momentum via another process (interaction with phonons)

Indirect Gap

Poor light emitter. e.g: Si, Ge



Silicon and III-V semiconductors

Silicon is by far the most prevalent semiconductor material. It readily forms a 4-fold covalently bonded lattice with other silicon atoms. Under certain conditions near perfect large scale crystals can be produced.

As a semiconductor it has good mobility values for both electrons and holes. Also it has a very long minority carrier lifetime, which is an asset for certain devices e.g: photodetectors.

Optically, however, it is an indirect gap material with weak absorption and almost zero emission.

Other properties

- Very abundant, unlike many other semiconductor materials.
- May be refinable to a very high purity (<ppb impurity)
- Excellent mechanical properties, giving the ultimate in crystal quality, low defect levels, surface finish quality etc.

Silicon and III-V semiconductors

- Wide range of well behaved dopants, eg: P, Sb, B
- Good thermal properties, important for heat transfer
- SiO_2 is an excellent dielectric, easily formed, stable, high ϵ

Si limitations

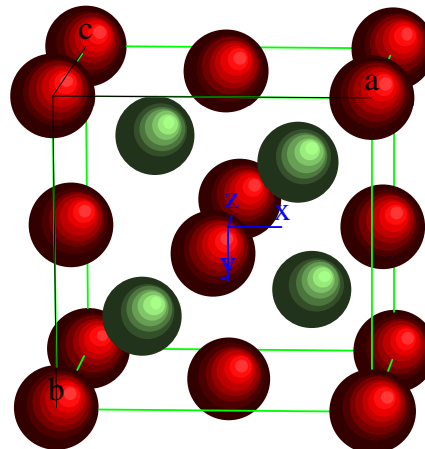
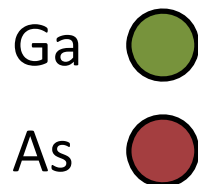
- Si electron mobility is not the best and the hole mobility is rather low. Many other materials with significantly better mobility values
- Si bandgap (1.1eV) is relatively low. Not well suited for high temperature applications
- No significant optical emission (no Si laser or LED)
- Relatively high temperature processing- high thermal budget

Silicon and III-V semiconductors

III-V semiconductors are made up of combinations of group III and group IV elements

Simple binary examples include GaAs, InP, GaN, InSb

GaAs is a 50:50 compound Ga & As. The 3 bonding electrons from Ga are shared with 5 from As to create a structure very similar to 4-fold covalent Si.



II	III	IV	V	VI
	5 B 10.81	6 C 12.01	7 N 14.01	8 O 16.00
	13 Al 26.98	14 Si 28.09	15 P 30.97	16 S 32.07
30 Zn 65.41	31 Ga 69.72	32 Ge 72.64	33 As 74.92	34 Se 78.96
48 Cd 112.4	49 In 114.8	50 Sn 118.7	51 Sb 121.8	52 Te 127.6
80 Hg 200.6	81 Tl 204.4	82 Pb 207.2	83 Bi 209.0	84 Po (209)

Silicon and III-V semiconductors

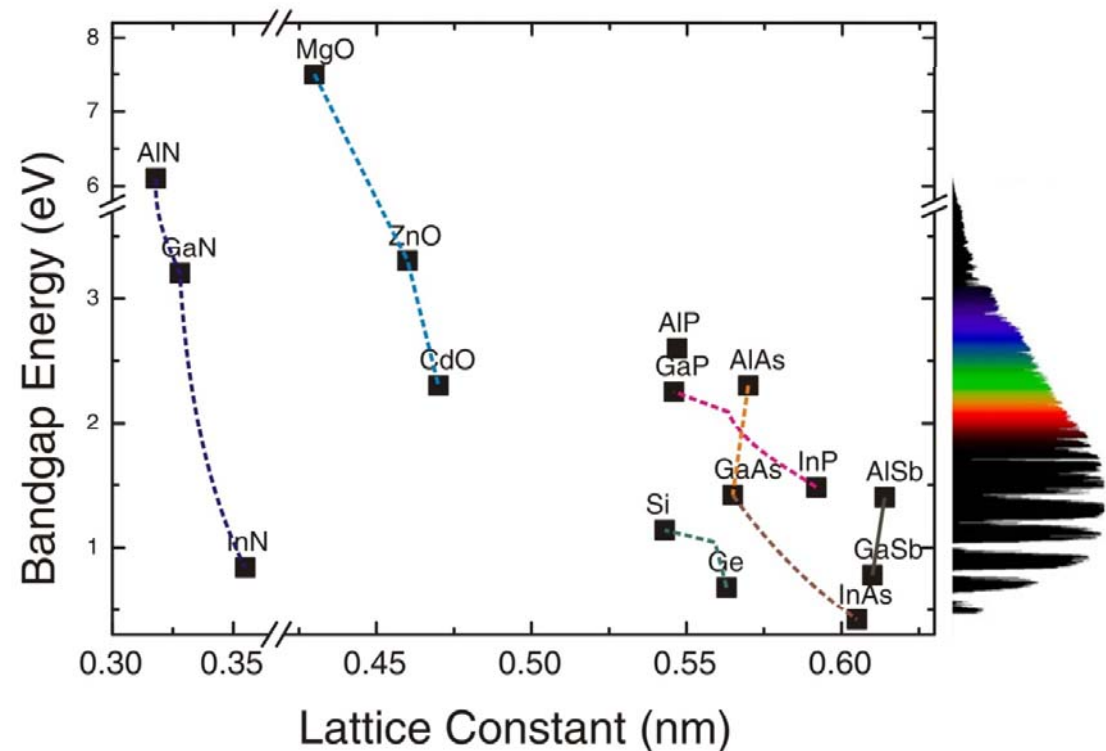
A range of binary III-V materials exists, with different band gaps and electronic properties.

We may further mix different group III and different group V materials together to form ternary and quaternary compounds compounds, covering an even wider range of band gaps.

Examples include InGaAs, a mixture of InAs and GaAs.

Strictly this is

$(\text{In}_x\text{Ga}_{1-x})_{0.5}(\text{As})_{0.5}$ but normally we drop the 0.5 and call this $\text{In}_x\text{Ga}_{1-x}\text{As}$



Silicon and III-V semiconductors

Quaternary materials include compounds such as InGaAsP $(\text{In}_x\text{Ga}_{1-x})_{.5}(\text{As}_y\text{P}_{1-y})_{.5}$ or simply $\text{In}_x\text{Ga}_{1-x}\text{As}_y\text{P}_{1-y}$.

The properties of III-V semiconductors are very diverse, but include

- Very low (eg: InSb) or very high (eg: AlN) band gaps
- Generally very high electron mobility compared to Si
- Generally higher saturation velocity compared to Si
- Often these are direct gap materials, which give strong optical absorption and emission (suitable for LEDs, Lasers etc)

III-V materials are part of a family of **compound semiconductors**.

There are other compounds of use including SiGe and SiC (IV-IV) semiconductors and compounds such as ZnO and CdS which are II-VI semiconductors. Note always the valency of 4 is preserved.

Heterojunctions

Heterojunctions are comprised of junctions between two different semiconductor materials

This can occur if the crystal structure is of the same type and the crystal dimensions (lattice constants) are similar

Si & Ge and GaAs & AlAs form two very common heterojunction families. They have the same crystal structure and very similar lattice constants. Because of this they can mix freely in different ratios.

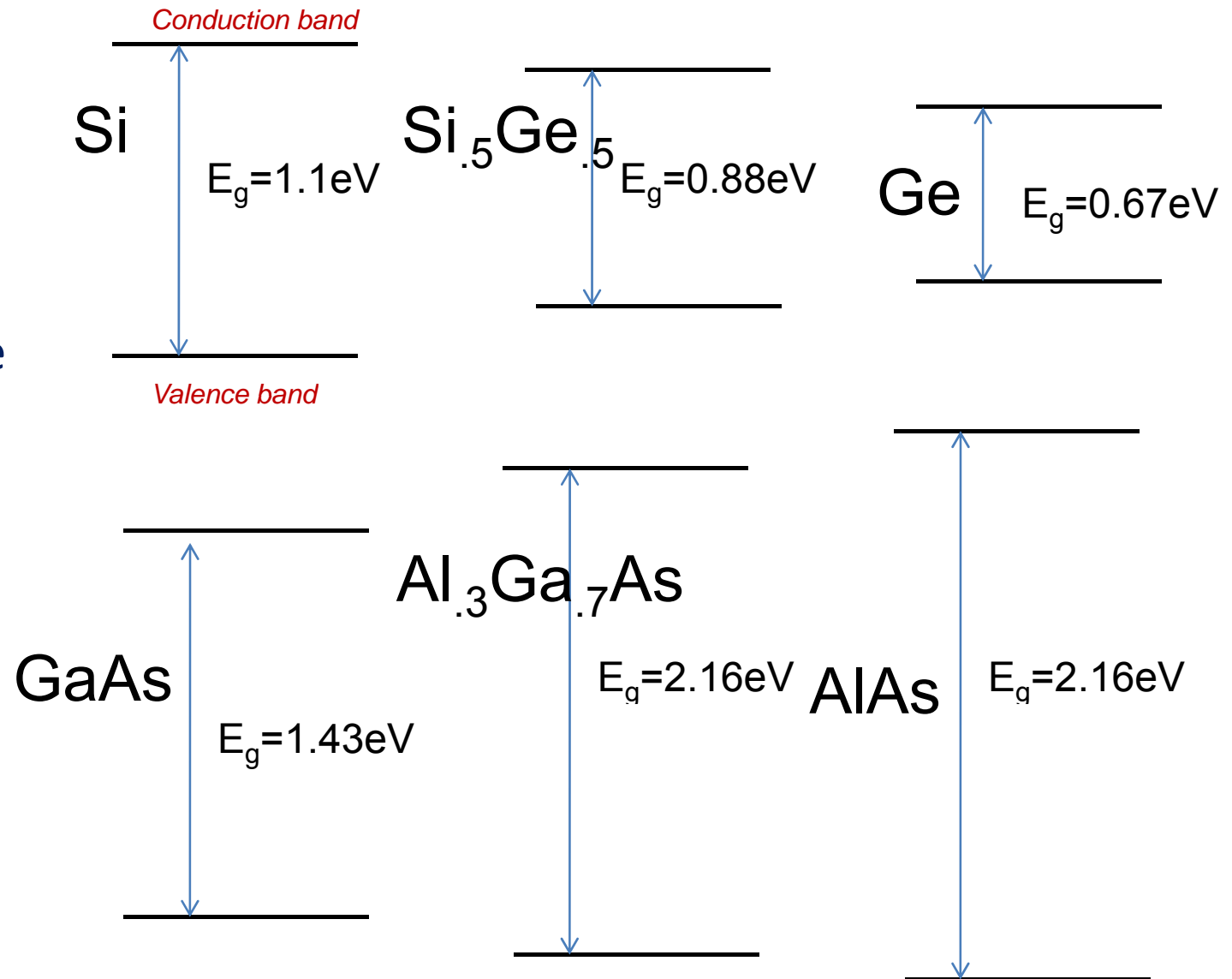
e.g: $\text{Si}_{.5}\text{Ge}_{.5}$ is a 50% mixture of silicon and germanium

$\text{Al}_{.3}\text{Ga}_{.7}\text{As}$ is a 30% mixture of AlAs with 70% GaAs. Strictly this should be written as $(\text{AlAs})_{.3}(\text{GaAs})_{.7}$.

The properties of these alloys, such as band gap, effective mass, mobility etc is usually well-approximated by a linear interpolation between the two end members (Vegard's law)

Heterojunctions

Si_{0.5}Ga_{0.5} has a band gap half way between that of Si and Ga. Its effective mass, mobility, saturation velocity etc are also well predicted by Vegard's law



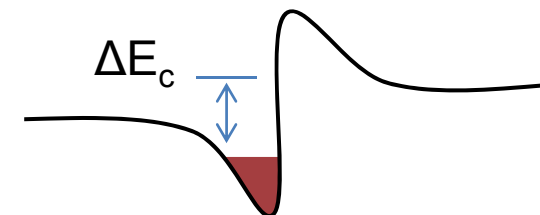
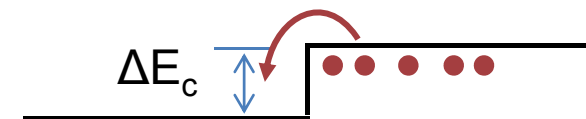
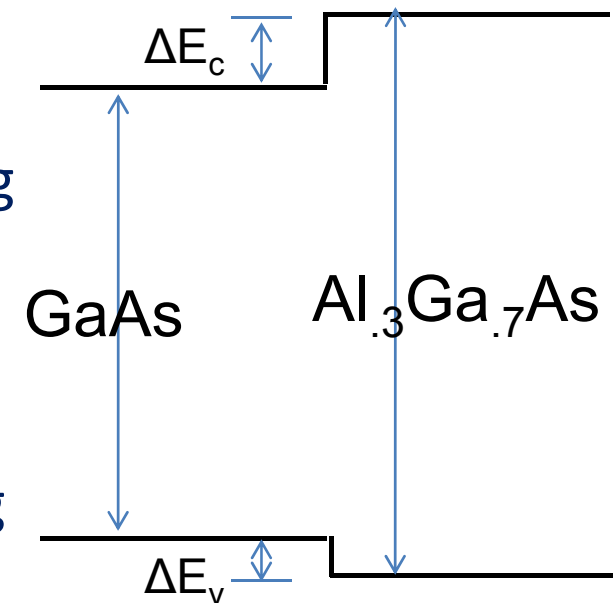
Heterojunctions

In a heterojunction the bands align according to the electron affinity of the materials, leaving a conduction and valance band discontinuity .

The band gap of the AlGaAs is split according to $E_{g_{\text{AlGaAs}}} = E_{g_{\text{GaAs}}} + \Delta E_c + \Delta E_v$

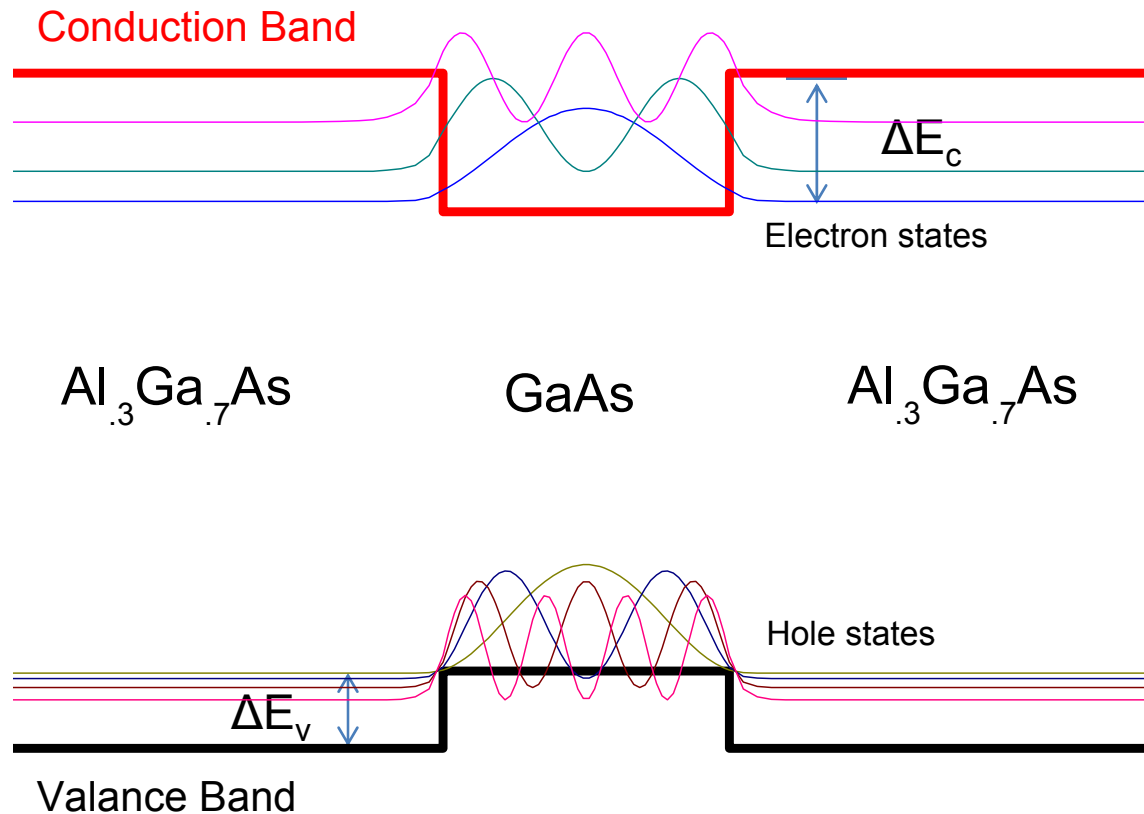
The discontinuities present barriers for carrier transport which can be exploited in the Heterojunction Bipolar Transistor (HBT)

We can also dope the heterojunction, eg: electrons will move to the lower band gap leaving the ionised donors behind. This is used in the High Electron Mobilty Transistor (HEMT)



Heterojunctions

With two heterojunctions we create a quantum well

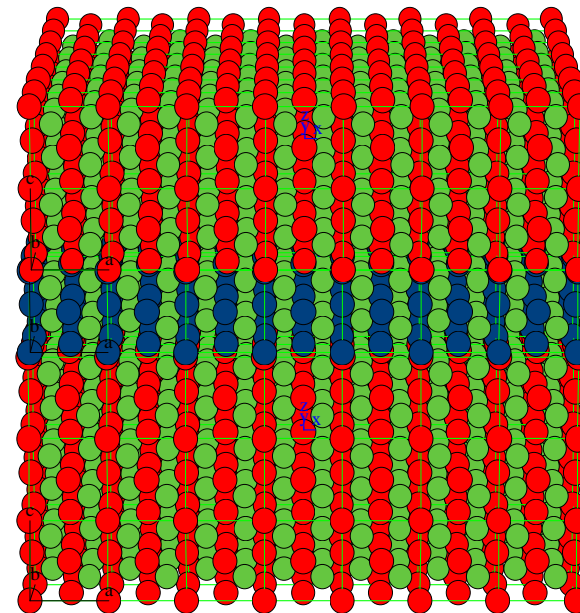
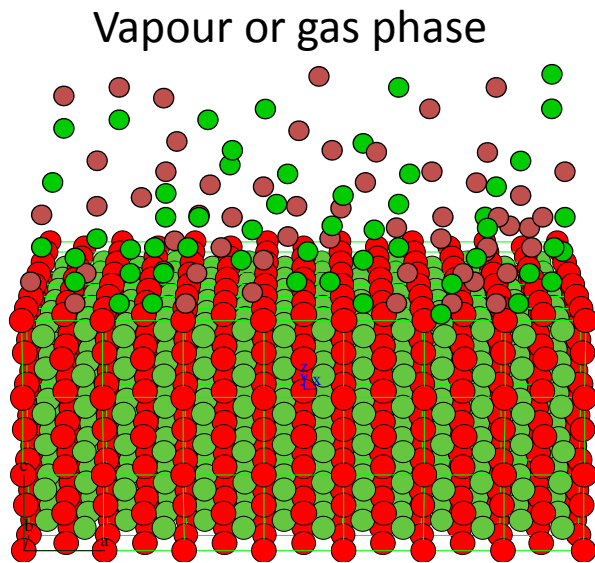


Electrons and holes in confined potential wells with properties determined by quantum mechanics, not by bulk properties

Heterojunctions

The formation of heterojunctions normally needs epitaxial growth methods such as MBE or MOCVD.

A switch of elemental species is performed to create layers with different band gap



Heterojunctions are incorporated in a large number of modern electronic devices and are particularly important for high speed.