CHAPTER 2
ENERGY BANDS AND EFFECTIVE MASS

- Semiconductors, insulators and metals
- Semiconductors
- Insulators
- Metals
- The concept of effective mass

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The electrical properties of metals and insulators are well known to all of us.

Everyday experience has already taught us a lot about the electrical properties of metals and insulators.

But the same cannot be said about “semiconductors”.

What happens when we connect a battery to a piece of a silicon; would it conduct well? or would it act like an insulator?
The name “semiconductor” implies that it conducts somewhere between the two cases (conductors or insulators).

Conductivity: $\sigma$

\[
\begin{align*}
\sigma_{\text{metals}} & \sim 10^{10} /\Omega\text{-cm} \\
S/C & \\
\sigma_{\text{insulators}} & \sim 10^{-22} /\Omega\text{-cm}
\end{align*}
\]

The conductivity ($\sigma$) of a semiconductor (S/C) lies between these two extreme cases.
The electrons surrounding a nucleus have certain well-defined energy-levels. 

Electrons don’t like to have the same energy in the same potential system. 

The most we could get together in the same energy-level was two, provided they had opposite spins. This is called **Pauli Exclusion Principle**.
The difference in energy between each of these smaller levels is so tiny that it is more reasonable to consider each of these sets of smaller energy-levels as being continuous *bands* of energy, rather than considering the enormous number of discrete individual levels.

Each *allowed band* is separated from another one by a *forbidden band*.

Electrons can be found in *allowed bands* but they cannot be found in *forbidden bands*.
**Consider 1 cm$^3$ of Silicon. How many atoms does this contain?**

**Solution:**

The atomic mass of silicon is 28.1 g which contains Avagadro’s number of atoms.

Avagadro’s number $N$ is $6.02 \times 10^{23}$ atoms/mol.

The density of silicon: $2.3 \times 10^3$ kg/m$^3$

so 1 cm$^3$ of silicon weighs 2.3 gram and so contains

$$
\frac{6.02 \times 10^{23}}{28.1} \times 2.3 = 4.93 \times 10^{22} \text{ atoms}
$$

This means that in a piece of silicon just one cubic centimeter in volume, each electron energy-level has split up into $4.93 \times 10^{22}$ smaller levels!
Semiconductor, Insulators, Conductors ::

Full band

All energy levels are occupied by electrons

Empty band

All energy levels are empty (no electrons)

Both full and empty bands do not partake in electrical conduction.
At low temperatures the valance band is *full*, and the conduction band is empty.

Recall that a full band can not conduct, and neither can an empty band.

At low temperatures, s/c’s do not conduct, they behave like insulators.

The *thermal energy* of the electrons sitting at the top of the full band is much lower than that of the *Eg at low temperatures*. 
Assume some kind of energy is provided to the electron (valence electron) sitting at the top of the valance band.

This electron gains energy from the applied field and it would like to move into higher energy states.

This electron contributes to the conductivity and this electron is called as a conduction electron.

At 0°C, electron sits at the lowest energy levels. The valance band is the highest filled band at zero kelvin.
When enough energy is supplied to the e⁻ sitting at the top of the valance band, e⁻ can make a transition to the bottom of the conduction band.

When electron makes such a transition it leaves behind a missing electron state.

This missing electron state is called as a hole.

Hole behaves as a positive charge carrier.

Magnitude of its charge is the same with that of the electron but with an opposite sign.
Conclusions

- Holes contribute to current in *valance band* (VB) as e⁻’s are able to create current in *conduction band* (CB).

- Hole is *not* a free particle. It can only exist within the crystal. A hole is simply a vacant electron state.

- A transition results in an equal number of e⁻ in CB and holes in VB. This is an important property of *intrinsic*, or *undoped s/c’s*. For *extrinsic*, or *doped*, semiconductors this is no longer true.
After transition, the valance band is now no longer full, it is *partly filled* and may conduct electric current.

- The *conductivity* is due to both electrons and holes, and this device is called a bipolar conductor or bipolar device.
What kind of excitation mechanism can cause an e\(^-\) to make a transition from the top of the valance band (VB) to the minimum or bottom of the conduction band (CB) ?

**Answer:**

- Thermal energy ?
- Electrical field ?
- Electromagnetic radiation ?

Energy band diagram of a s/c at a finite temperature.

To have a partly field band configuration in a s/c , one must use one of these excitation mechanisms.
1- Thermal Energy:

\[ \text{Thermal energy} = k \times T = 1.38 \times 10^{-23} \text{ J/K} \times 300 \text{ K} = 25 \text{ meV} \]

\[ \text{Excitation rate} = \text{constant} \times \exp\left(-\frac{E_g}{kT}\right) \]

Although the thermal energy at room temperature, \( RT \), is very small, i.e. 25 meV, a few electrons can be promoted to the CB.

*Electrons can be promoted to the CB by means of thermal energy.*

This is due to the exponential increase of excitation rate with increasing temperature.

*Excitation rate is a strong function of temperature.*
For low fields, this mechanism doesn’t promote electrons to the CB in common s/c’s such as Si and GaAs.

An electric field of $10^{18}$ V/m can provide an energy of the order of 1 eV. This field is enormous.

So, the use of the electric field as an excitation mechanism is not useful way to promote electrons in s/c’s.
3- Electromagnetic Radiation:

\[ E = h\nu = h\frac{c}{\lambda} = \left(6.62 \times 10^{-34} \text{ J-s}\right) \times \left(3 \times 10^8 \text{ m/s}\right) / \lambda(\text{m}) \Rightarrow E(\text{eV}) = \frac{1.24}{\lambda(\text{in } \mu\text{m})} \]

\[ h = 6.62 \times 10^{-34} \text{ J-s} \]
\[ c = 3 \times 10^8 \text{ m/s} \]
\[ 1 \text{ eV} = 1.6 \times 10^{-19} \text{ J} \]

\[ \text{for Silicon} \quad E_g = 1.1 \text{ eV} \quad \lambda(\mu\text{m}) = \frac{1.24}{1.1} = 1.1 \mu\text{m} \]

To promote electrons from VB to CB Silicon, the wavelength of the photons must 1.1 \mu m or less.
The converse transition can also happen.

- An electron in CB recombines with a hole in VB and generate a photon.
- The energy of the photon will be in the order of Eg.
- If this happens in a direct band-gap s/c, it forms the basis of LED’s and LASERS.
The magnitude of the band gap determines the differences between insulators, s/c’s and metals.

The excitation mechanism of thermal is not a useful way to promote an electron to CB even the melting temperature is reached in an insulator.

Even very high electric fields is also unable to promote electrons across the band gap in an insulator.

Wide band gaps between VB and CB.
These two bands look like as if partly filled bands and it is known that partly filled bands conduct well.

This is the reason why metals have high conductivity.

No gap between *valance band* and *conduction band*
The Concept of Effective Mass:

Comparing

<table>
<thead>
<tr>
<th>Free ( e^- ) in vacuum</th>
<th>An ( e^- ) in a crystal</th>
</tr>
</thead>
<tbody>
<tr>
<td>In an electric field</td>
<td>In an electric field</td>
</tr>
<tr>
<td>( m_o = 9.1 \times 10^{-31} )</td>
<td>In a crystal</td>
</tr>
<tr>
<td>Free electron mass</td>
<td></td>
</tr>
<tr>
<td></td>
<td>( m = ? )</td>
</tr>
<tr>
<td></td>
<td>( m^* \rightarrow \text{effective mass} )</td>
</tr>
</tbody>
</table>

- If the same magnitude of electric field is applied to both electrons in vacuum and inside the crystal, the electrons will accelerate at a different rate from each other due to the existence of different potentials inside the crystal.
- The electron inside the crystal has to try to make its own way.
- So the electrons inside the crystal will have a different mass than that of the electron in vacuum.
- This altered mass is called as an effective-mass.
What is the expression for $m^*$

- Particles of electrons and holes behave as a wave under certain conditions. So one has to consider the de Broglie wavelength to link particle behaviour with wave behaviour.
- Particles such as electrons and waves can be diffracted from the crystal just as X-rays.
- Certain electron momentum is not allowed by the crystal lattice. This is the origin of the energy band gaps.

$$n\lambda = 2d \sin\theta$$

- $n$ = the order of the diffraction
- $\lambda$ = the wavelength of the X-ray
- $d$ = the distance between planes
- $\theta$ = the incident angle of the X-ray beam
\( n\lambda = 2d \)  \( \quad \text{(1)} \)

The waves are standing waves

\( \lambda = \frac{2\pi}{k} \)

is the propagation constant

The momentum is

\[ P = \hbar k \]  \( \quad \text{(2)} \)

The energy of the free electron can be related to its momentum

\[ E = \frac{P^2}{2m} \]

free e\textsuperscript{-} mass, \( m_0 \)

\[ E = \frac{\hbar^2}{2m} \frac{1}{\lambda^2} = \frac{\hbar^2}{2m} \frac{k^2}{(2\pi)^2} \]

\[ \hbar = \frac{\hbar}{2\pi} E = \frac{\hbar^2 k^2}{2m} \]

The energy of the free e\textsuperscript{-} is related to the k

By means of equations (1) and (2) certain e\textsuperscript{-} momenta are not allowed by the crystal. The velocity of the electron at these momentum values is zero.

E versus k diagram is a parabola.

Energy is continuous with k, i.e., all energy (momentum) values are allowed.

E versus k diagram or Energy versus momentum diagrams
To find effective mass, $m^*$

We will take the derivative of energy with respect to $k$:

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

Then:

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

- $m^*$ is determined by the curvature of the E-k curve.
- $m^*$ is inversely proportional to the curvature.

Change $m^*$ instead of $m$.

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

This formula is the effective mass of an electron inside the crystal.
Direct an indirect-band gap materials:

For a *direct-band gap material*, the minimum of the *conduction band* and maximum of the *valance band* lies at the same momentum, \( k \), values.

- When an electron sitting at the bottom of the \( \text{CB} \) recombines with a hole sitting at the top of the \( \text{VB} \), there will be no change in momentum values.

- Energy is conserved by means of emitting a photon, such transitions are called as *radiative transitions*. 
For an indirect-band gap material; the minimum of the CB and maximum of the VB lie at different k-values.

When an e\textsuperscript{-} and hole recombine in an indirect-band gap s/c, phonons must be involved to conserve momentum.

**Phonon**

- Atoms vibrate about their mean position at a finite temperature. These vibrations produce vibrational waves inside the crystal.
- Phonons are the quanta of these vibrational waves. Phonons travel with a velocity of sound.
- Their wavelength is determined by the crystal lattice constant. Phonons can only exist inside the crystal.
- The transition that involves phonons without producing photons are called \textit{nonradiative (radiationless) transitions}.

- These transitions are observed in an \textit{indirect band gap} s/c and result in inefficient photon producing.

- So in order to have efficient LED’s and LASER’s, one should choose materials having direct band gaps such as compound s/c’s of GaAs, AlGaAs, etc…
For GaAs, calculate a typical (band gap) photon energy and momentum, and compare this with a typical phonon energy and momentum that might be expected with this material.

<table>
<thead>
<tr>
<th><strong>photon</strong></th>
<th><strong>phonon</strong></th>
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<tbody>
<tr>
<td>(E(\text{photon}) = E_g(\text{GaAs}) = 1.43 \text{ ev})</td>
<td>(E(\text{phonon}) = h \frac{\nu}{\lambda} = \frac{h c}{\lambda})</td>
</tr>
<tr>
<td>(E(\text{photon}) = h \nu = h c / \lambda)</td>
<td>(E(\text{phonon}) = h \nu_s / a_0)</td>
</tr>
<tr>
<td>(c = 3 \times 10^8 \text{ m/sec})</td>
<td>(\lambda (\text{phonon}) \sim a_0 = \text{lattice constant} = 5.65 \times 10^{-10} \text{ m})</td>
</tr>
<tr>
<td>(P = h / \lambda) (h = 6.63 \times 10^{-34} \text{ J-sec})</td>
<td>(V_s = 5 \times 10^3 \text{ m/sec (velocity of sound)})</td>
</tr>
<tr>
<td>(\lambda (\text{photon}) = 1.24 / 1.43 = 0.88 \mu\text{m})</td>
<td>(E(\text{phonon}) = h \nu_s / a_0 = 0.037 \text{ eV})</td>
</tr>
<tr>
<td>(P(\text{photon}) = h / \lambda = 7.53 \times 10^{-28} \text{ kg-m/sec})</td>
<td>(P(\text{phonon}) = h / \lambda = h / a_0 = 1.17 \times 10^{-24} \text{ kg-m/sec})</td>
</tr>
</tbody>
</table>
- Photon energy = 1.43 eV
- Phonon energy = 37 meV
- Photon momentum = $7.53 \times 10^{-28}$ kg-m/sec
- Phonon momentum = $1.17 \times 10^{-24}$ kg-m/sec

Photons carry large energies but negligible amount of momentum.

On the other hand, phonons carry very little energy but significant amount of momentum.
Positive and negative effective mass

The sign of the effective mass is determined directly from the sign of the curvature of the E-k curve.

- The curvature of a graph at a minimum point is a positive quantity and the curvature of a graph at a maximum point is a negative quantity.

- Particles (electrons) sitting near the minimum have a **positive effective mass**.

- Particles (holes) sitting near the valence band maximum have a **negative effective mass**.

- A negative effective mass implies that a particle will go *the wrong way* when an external force is applied.

\[
m^* = \frac{\hbar^2}{d^2 E/dk^2}
\]
Energy band structures of GaAs and Si
Band gap is the smallest energy separation between the valence and conduction band edges.

The smallest energy difference occurs at the same momentum value.

Direct band gap semiconductor

Energy band structure of GaAs
The smallest energy gap is between the top of the VB at $k=0$ and one of the CB minima away from $k=0$.

Indirect band gap semiconductor

- Band structure of AlGaAs?
- Effective masses of CB satellites?
- Heavy- and light-hole masses in VB?

Energy band structure of $Si$
direct transition

$E_g$
Direct transition
indirect transition

$E_g$
indirect transition