Lecture 6: Semiconductor Basics (Band Gap and density of states)

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Electrons and Holes

As seen from the previous lecture in the simplified 1D E-k diagram there are some bands at 0K that are completely filled with electrons and there are upper lying bands which are completely empty of electrons. None of these electrons can carry current. However, the picture completely changes when some electrons from the completely bands are excited to the completely empty bands.

The electrons that are in the almost empty band can now be accelerated to higher momentum and energy and therefore conduct electricly, etc. in this band called the conduction band, and the effective mass that can be applied to classical formulae is given by:

\[ \frac{dE}{dk} = q \mathcal{F} \]

\[ \frac{d}{dt} \left( \frac{\hbar k}{m^*} \right) = \frac{q \mathcal{F}}{\hbar}, m^* = \frac{\hbar^2 k}{dE / dk} \]

The electrons that are in the almost filled band can now be accelerated to higher momentum and energy and therefore conduct electricity, etc. However, the curvature of the band (E-p dispersion relationship) is in the opposite direction to that of the almost empty band. Hence the picture is that the absence of electrons (vacancies) are moving in the opposite direction to that of electrons with the application of electric field, which should be true for a +ve charged particle. Hence the +ve charged vacancy (Hole) should have an effective mass that which is also –ve as is given by:

\[ v_g = \mu \mathcal{F}, \quad \mu \text{ is called the mobility} \]

When diffusion of carriers is also present it is assumed

\[ \frac{D}{\mu} = \frac{kT}{q} \]
Semiconductor Materials for low dispersion, low loss fiber wavelengths

The shaded area comprises of alloys of GaP, GaAs, InP, and InAs and hence are called Quarternary alloys of the type \( \text{In}_x\text{Ga}_{1-x}\text{As}_y\text{P}_{1-y} \)

Any parameter \( P(x,y) \) can be found through Vegard’s Law (linear interpolation) such as:

\[
P(x,y) = (1-x)y.P_{\text{GaAs}} + (1-x)(1-y).P_{\text{GaP}} + xy.P_{\text{InAs}} + x(1-y).P_{\text{InP}}
\]

However, if one considers only those compositions which are lattice matched to that of InP \((a=0.5869\text{nm})\) then the constraint is \( x=1-0.48y \).

The InP lattice matched band gaps are incorrect due to bowing in linear interpolation and hence are given in (eV) by:

\[
E_g(4.2K)=1.425-0.7668y+0.149y^2
\]

\[
E_g(298K)=1.35-0.775y+0.149y^2
\]
Heterostructure Band

Junction of two dissimilar semiconductors (Doping as well as Band Gap)

Quaternary alloys of the type III$_x$-III$_{1-x}$-V$_y$-V$_{1-y}$

F(x,y) for an alloy A$_x$-B$_{1-x}$-C$_y$-D$_{1-y}$

P(x,y) = (1-x)yP(BC) + (1-x)(1-y)P(BD)
  + xyP(AC) + x(1-y)P(AD)

T$_{ABC}$ (x) = xB$_{AB}$ + (1-x)B$_{AC}$ - x(1-x)C$_{ABC}$

Alloys of the type A-B$_x$-C$_y$-D$_{1-x}$

Q(x,y) = \frac{xyT_{ABC}(u) + y(1-x-y)T_{ACD}(v) + x(1-x-y)T_{ABD}(w)}{xy + y(1-x-y) + x(1-x-y)}

φ = Work Function  \chi = Electron Affinity
Density of States in semiconductors

For a bound electron, the 3D Schrödinger is

\[ \nabla^2 \Psi + \frac{2m}{\hbar^2} (E - V) \Psi = 0 \]

where \( \Psi = \Psi(x, y, z) = (\text{constant}) e^{i \mathbf{k} \cdot \mathbf{r}} \)

And for \( 0 < x < a \)

\[ k = \sqrt{\frac{2mE}{\hbar^2}} \]

with \( \psi(x + R, y, z) = \psi(x, y, z) \)

And for the \( y \)- and \( z \)-directions.

Using separation of Variable technique

\[ \psi(x, y, z) = \psi_x(x) \cdot \psi_y(y) \cdot \psi_z(z) \]

\[ \frac{d^2 \psi_x(x)}{dx^2} + k_x^2 \psi_x(x) = 0, \quad \frac{d^2 \psi_y(y)}{dy^2} + k_y^2 \psi_y(y) = 0, \quad \frac{d^2 \psi_z(z)}{dz^2} + k_z^2 \psi_z(z) = 0 \]

\( k_x^2 + k_y^2 + k_z^2 = k^2 \)

For \( \psi_x(x + R) = \psi_x(x) \)

And similarly for the \( y \)- and \( z \)-directions.

Remember reduction of Brillouin Zone in Kronig-Penny Model

\[ \Delta k = \frac{2\pi n}{(a + b)} \]

\[ k_x = \frac{2\pi}{R} n_x, k_y = \frac{2\pi}{R} n_y, k_z = \frac{2\pi}{R} n_z \]

Or \( \psi_n = A \exp \left[ j \frac{2\pi}{R} (n_x x + n_y y + n_z z) \right] \)

Where \( n \)'s are integer factors in each direction, \( x, y, z \), and

\[ A \text{ is a normalizing factor and } V \text{ is the volume of the cube of sides 'R'} \]

\[ E_n = \frac{\hbar^2}{2m} \left( \frac{2\pi}{R} \right)^2 \left( n_x^2 + n_y^2 + n_z^2 \right) = \frac{(2\pi)^2 \hbar^2 n^2}{2mV^{2/3}} \]

\[ k_n^2 = \frac{(2\pi)^2}{V^{2/3}} n^2 \]
The volume per k-state is
\[ V_k = \frac{(2\pi)^3}{V} \]
\[ (k^2 = \frac{2mE}{\hbar^2}) \]
\[ E_n = \frac{\hbar^2 k_n^2}{2m} \]

Then the Momentum is given by
\[ p_n = \hbar k_n, \rightarrow p^2 = p_x^2 + p_y^2 + p_z^2 = 2mE \]

Or in the Momentum space diagram shown
\[ V_p = \hbar^3 (2\pi)^3 / V \]

The number of allowed energy states between the energy \( E \) and \( E + dE \) will be given by the volume in \( p \)-space for values within \( p \) and \( p + dp \) divided by the unit volume in \( p \)-space (Where a factor of 2 is due to Electron Spin being \( \pm \frac{1}{2} \)): \[ \Delta V_p = 2 \times 4\pi p^2 dp, \]
\[ 2pdp = 2mdE : \Delta V_p = 8\pi p.mdE = 8\pi \sqrt{2mE} . mdE \]

The number of available quantum states is \[ \Delta V_p / V_p \]
\[ \therefore N(E)dE = 8\pi \sqrt{2mE} . mdE / \left[ \hbar^3 (2\pi)^3 / V \right] \]

Or per unit volume 'V'
\[ N(E) = \frac{1}{2\pi^2} \left( \frac{2m}{\hbar^2} \right)^{3/2} E^{1/2} \]

Hence for a 3D lattice per unit volume having an effective mass of electrons and holes in the conduction band and valence bands, respectively
\[ N_e(E) = \left( \frac{2m_e^*}{\hbar^2} \right)^{3/2} \frac{1}{2\pi^2} \sqrt{E - E_c} \]
\[ \text{and} \]
\[ N_h(E) = \left( \frac{2m_h^*}{\hbar^2} \right)^{3/2} \frac{1}{2\pi^2} \sqrt{E_v - E} \]
Similarly for a 2D lattice the space between \( k \) and \( k+dk \) is: \( 2\pi k dk \)

\[
N_{2D}(E) dE = \frac{2}{(2\pi)^2} (2\pi k) dk = \left( \frac{m}{\pi \hbar^2} \right) dE
\]

Note that for \( n^{th} \) quantized state, the density of state would be

\[
n \left( \frac{m}{\pi \hbar^2} \right)
\]

Similarly for a 1D lattice the space between \( k \) and \( k+dk \) is: \( dk \)

And per unit volume 1D density of states is

\[
N_{1D}(E) dE = \frac{2}{(2\pi)} 2dk = \left( \frac{\sqrt{2m}}{\pi \hbar \sqrt{E}} \right) dE
\]

For a 0D lattice (quantum dot) the density of states is just a delta function

For 3D electrons in conduction band

\[
N_e = \left( \frac{2m_e^*}{\hbar^2} \right)^{3/2} \frac{1}{4\pi^2} \sqrt{E - E_c}
\]

And

\[
n_o = N_c f(E_c) \quad \text{where} \quad f(E) = \frac{1}{\exp((E-E_F)/kT) + 1}
\]

\[
n_o = \frac{1}{2\pi^2} \left( \frac{2m_e^*}{\hbar^2} \right)^{3/2} e^{E_F/kT} \int_{E_c}^{\infty} E^{1/2} e^{E/kT} dE
\]

For 3D holes in Valence band

\[
N_h = \left( \frac{2m_h^*}{\hbar^2} \right)^{3/2} \frac{1}{4\pi^2} \sqrt{E_v - E}
\]

\[
\text{Or} \quad n_o = \int_{E_c}^{\infty} N(E) f(E) dE
\]

\[
\therefore n_o = 2 \left( \frac{2\pi m^* kT}{\hbar^2} \right)^{3/2} e^{E_F/kT}
\]
Review Questions:

1. Find the composition of InGaAsP alloy lattice matched to InP for which the band gap is 0.85eV.

2. Check the band shape of an indirect semiconductor and that of a direct band gap semiconductor. Justify whose electron effective mass would be larger.

3. Look at the shapes of the conduction band and the valence band of a direct band gap semiconductor. For electrons in the conduction band and holes in the valence band, which should have a larger effective mass?

4. Take $m_e^* = 0.07m_o$ and $m_h^* = 0.7m_o$ and plot the density of states for both. How similar are they?

5. Note that there are two valence bands at the $\Gamma$-point ($k=0$). Their curvatures are very different. Which should be called Heavy Hole (hh) and which should be called Light Hole (lh)?

6. Do a similar exercise as that in the previous lecture and find the quantization energies for $a=5nm$, $b=200nm$, $m_e^* = 0.07m_o$, and $m_h^* = 0.7m_o$.