Lecture 4

Density of States and Fermi Energy Concepts

Reading:
(Cont’d) Pierret 2.1-2.6
How do electrons and holes populate the bands?

Density of States Concept

Quantum Mechanics tells us that the number of available states in a cubic cm per unit of energy, the density of states, is given by:

$$g_c(E) = \frac{m^*_n \sqrt{2m^*_n (E - E_c)}}{\pi^2 \hbar^3}, \quad E \geq E_c$$

$$g_v(E) = \frac{m^*_p \sqrt{2m^*_p (E_v - E)}}{\pi^2 \hbar^3}, \quad E \leq E_v$$

unit  $\equiv \left[ \frac{\text{Number of States}}{m^3} \right] / \text{Joule} \Rightarrow \left[ \frac{\text{Number of States}}{cm^3} \right] / eV$
How do electrons and holes populate the bands?

Density of States Concept

Thus, the number of states per cubic centimeter between energy $E'$ and $E'+dE$ is

\[
g_c(E')dE \text{ if } E' \geq E_c \quad \text{and,} \\
g_v(E')dE \text{ if } E' \leq E_v \quad \text{and,} \\
0 \text{ otherwise}
\]
How do electrons and holes populate the bands?

Probability of Occupation (Fermi Function) Concept

Now that we know the number of available states at each energy, how do the electrons occupy these states?

We need to know how the electrons are “distributed in energy”.

Again, Quantum Mechanics tells us that the electrons follow the “Fermi-distribution function”.

\[
f(E) = \frac{1}{1 + e^{(E - E_F)/kT}}
\]

where \( k \equiv \text{Boltzman constant}, T \equiv \text{Temperature in Kelvin} \)

and \( E_F \equiv \text{Fermi energy} (\sim \text{average energy of our electrons in the crystal}) \)

\[
f(E) \text{ is the probability that a state at energy } E \text{ is occupied}
\]

\[
1 - f(E) \text{ is the probability that a state at energy } E \text{ is unoccupied}
\]
An Aside about the fermi energy:

• If the material had an imbalance of average electron energy from one side to another, electrons would flow from the region of high energy toward the region of low energy to balance out the average energy. Thus, gradients in the average energy would result in a current (flow of electrons) until the energy balance was satisfied. If an outside force maintained such an imbalance in energy from one region to another, a continuous current would result (see “quasi-fermi” energy concept introduced later).

• When “assembling our crystal”, if we brought extra electrons into the crystal such as in the case of donor doping, we have to do more work to introduce the extra valence electrons. Thus, the average electron energy would increase compared to the intrinsic doped case.

• When “assembling our crystal”, if we brought fewer electrons into the crystal such as in the case of acceptor doping, we have to do less work to introduce the fewer valence electrons. Thus, the average electron energy would decrease compared to the intrinsic doped case.
How do electrons and holes populate the bands?

Probability of Occupation (Fermi Function) Concept

At T=0K, occupancy is “digital”: No occupation of states above $E_F$ and complete occupation of states below $E_F$

At T>0K, occupation probability is reduced with increasing energy.

$f(E=E_F) = 1/2$ regardless of temperature.
How do electrons and holes populate the bands?

Probability of Occupation (Fermi Function) Concept

At T=0K, occupancy is “digital”: No occupation of states above $E_F$ and complete occupation of states below $E_F$

At T>0K, occupation probability is reduced with increasing energy.

$f(E=E_F) = 1/2$ regardless of temperature.

At higher temperatures, higher energy states can be occupied, leaving more lower energy states unoccupied ($1-f(E)$).
How do electrons and holes populate the bands?

Probability of Occupation (Fermi Function) Concept – Si Example

\[ f(E) = \frac{1}{1 + e^{\frac{(E-E_F)}{kT}}} \]

For \( E > (E_f + 3kT) \):
\[ f(E) \sim e^{-\frac{(E-E_f)}{kT}} \sim 0 \]

For \( E < (E_f - 3kT) \):
\[ f(E) \sim 1 - e^{-\frac{(E-E_f)}{kT}} \sim 1 \]

\( E_f = 0.55 \text{ eV} \)

\( T=10 \text{ K}, \ kT=0.00086 \text{ eV} \)
\( T=300 \text{K}, \ kT=0.0259 \)
\( T=450 \text{K}, \ kT=0.039 \)
How do electrons and holes populate the bands?

Probability of Occupation (Fermi Function) Concept – Si Example

\[
f(E) = \frac{1}{1 + e^{\frac{(E-E_F)}{kT}}}
\]

\[\text{T}=450\text{K}, \ kT=0.039\]

Intrinsic Case

Valence Band States

Conduction Band States

- Insignificant emptying of valance band states
- Insignificant occupation of conduction band states
- No States in the bandgap

\[E_f=0.55\text{ eV}\]
How do electrons and holes populate the bands?

Probability of Occupation (Fermi Function) Concept – Si Example

\[ f(E) = \frac{1}{1 + e^{(E-E_F)/kT}} \]

\[ E=1.05 \text{ eV} \]

\[ T=450K, \ kT=0.039 \]

**Donor Case**

- Significant occupation of conduction band states
- No States in the bandgap

Donor Doped
How do electrons and holes populate the bands?

Probability of Occupation (Fermi Function) Concept – Si Example

\[ f(E) = \frac{1}{1 + e^{\frac{(E-E_F)/kT}{kT}}} \]

\[ T=450K, \ kT=0.039 \]

**Accepter Case**

- Significant emptying of valence band states
- \( E_f=0.05 \text{ eV} \)
- Donor Doped

Valence Band States

Conduction Band States

No States in the bandgap
How do electrons and holes populate the bands?

Probability of Occupation

Thus, the density of electrons (or holes) occupying the states in energy between E and E+dE is:

- Electrons/cm$^3$ in the conduction band between Energy E and E+dE:
  \[g_c(E) f(E) \, dE \quad \text{if} \quad E \geq E_c \quad \text{and},\]

- Holes/cm$^3$ in the valence band between Energy E and E+dE:
  \[g_v(E) [1 - f(E)] \, dE \quad \text{if} \quad E \leq E_v \quad \text{and},\]

0 otherwise
How do electrons and holes populate the bands?

Band Occupation

Figure 2.16 Carrier distributions (not drawn to scale) in the respective bands when the Fermi level is positioned (a) above midgap, (b) near midgap, and (c) below midgap. Also shown in each case are coordinated sketches of the energy band diagram, density of states, and the occupancy factors (the Fermi function and one minus the Fermi function).
How do electrons and holes populate the bands?

Intrinsic Energy (or Intrinsic Level)

$E_f$ is said to equal $E_i$ (intrinsic energy) when...

$E_f$ is above midgap

$E_f$ is near midgap

$E_f$ is below midgap

Figure 2.16 Carrier distributions (not drawn to scale) in the respective bands when the Fermi level is positioned (a) above midgap, (b) near midgap, and (c) below midgap. Also shown in each case are coordinated sketches of the energy band diagram, density of states, and the occupancy factors (the Fermi function and one minus the Fermi function).
How do electrons and holes populate the bands?

Correction for the Presence of Additional Dopant States

Intrinsic:
Equal number of electrons and holes

n-type: more electrons than holes

p-type: more holes than electrons