Lecture 2 - Carrier Statistics in Equilibrium

February 8, 2007

Contents:

- 1. Conduction and valence bands, bandgap, holes
- 2. Intrinsic semiconductor
- 3. Extrinsic semiconductor
- 4. Conduction and valence band density of states

Reading assignment:

del Alamo, Ch. 2, §§2.1-2.4 (2.4.1)

Announcement:

Go to <u>http://ilab.mit.edu</u> and register. Select membership in the 6.720 group. You will need this to access the lab for the Device Characterization Projects.

Key questions

- What are these "energy band diagrams"?
- What are these "holes"?
- In a perfectly pure semiconductor, how many electrons and holes are there?
- Can one engineer the electron and hole concentrations in a semiconductor?

1. Conduction and valence bands, bandgap, holes



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"





Elements of energy band diagrams:

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



2. Intrinsic semiconductor

Define *intrinsic semiconductor*, or "ideal" semiconductor:

- perfectly crystalline (no perturbations to periodic lattice)
- perfectly pure (no foreign atoms)
- no surface effects

Question: How many electrons and holes are there in an intrinsic semiconductor in thermal equilibrium at a given temperature?

Answer requires fairly elaborate model [lecture 3], but key dependencies can be readily identified.

Define:

 $n_o \equiv$ equilibrium (free) electron concentration in conduction band $[cm^{-3}]$

 $p_o \equiv$ equilibrium hole concentration in valence band $[cm^{-3}]$

Certainly in intrinsic semiconductor:

$$n_o = p_o = n_i$$

$$n_i \equiv \text{intrinsic carrier concentration } [cm^{-3}]$$

Key dependencies of n_i :

• Temperature:

$$T \uparrow \Rightarrow n_i$$

• Bandgap:

$$E_g \uparrow \Rightarrow n_i$$

What is detailed form of dependencies?

Use analogy of chemical reactions.

Electron-hole formation can be thought of as chemical reaction:

$$bond \rightleftharpoons e^- + h^+$$

similar to water decomposition reaction:

$$H_2 O \rightleftharpoons H^+ + O H^-$$

Law-of-mass action relates concentration of reactants and reaction products. For water:

$$K = \frac{[H^+][OH^-]}{[H_2O]} \sim \exp(-\frac{E}{kT})$$

E is energy consumed or released in reaction.

This is a "thermally activated" process \Rightarrow rate of reaction limited by need to overcome energy barrier E (activation energy).

In analogy, for electron-hole formation:

$$K = \frac{n_o p_o}{[bonds]} \sim \exp(-\frac{E_g}{kT})$$

[bonds] is concentration of unbroken bonds.

Note: activation energy is E_q .

In general, relatively few bonds are broken. Hence:

$$[bonds] \gg n_o, p_o$$

and

$$[bonds] \simeq constant$$

Then:

$$n_o p_o \sim \exp(-\frac{E_g}{kT})$$

Two important results:

• First,

$$n_i \sim \exp(-\frac{E_g}{2kT})$$

As expected: $T \uparrow \Rightarrow n_i \uparrow$

$$E_g \uparrow \Rightarrow n_i \downarrow$$

To get prefactor, need detailed model [lecture 3].

Arrhenius plot for Si [experiments of Misiakos and Tsamakis, 1993]:



In Si at 300 K, $n_i \simeq 1.1 \times 10^{10} \ cm^{-3}$.

• Second important result:

$$n_o p_o = n_i^2$$

Equilibrium np product in a semiconductor at a certain temperature is a constant specific to the semiconductor.

3. Extrinsic semiconductor

Can electron and hole concentrations be engineered?

Insert *dopants* in substitutional positions in the lattice:

- **Donors**: introduce electrons to conduction band without introducing holes to valence band
- Acceptors: introduce holes to valence band without introducing electrons to conduction band

If any one carrier type overwhelms $n_i \Rightarrow \text{extrinsic semiconductor}$





Acceptor in Si, atom from column III (B):



Representation of donor and acceptor states in energy band diagram:



 $E_d, E_a \sim 40 - 60 \ meV$, for common dopants

 \Box Near room temperature, all dopants are ionized:

$$N_D^+ \simeq N_D$$

$$N_A^- \simeq N_A$$

Typical doping levels:

$$N_A, N_D \sim 10^{15} - 10^{20} \ cm^{-3}$$

\Box n-type semiconductor

$$n_o \simeq N_D$$

 $p_o \simeq \frac{n_i^2}{N_D}$

These equations are valid at intermediate temperatures.



 \Box p-type semiconductor

$$p_o \simeq N_A$$

 $n_o \simeq \frac{n_i^2}{N_A}$

4. Conduction and valence band density of states

Image removed due to copyright restrictions.

Figure 1b) on p. 468 in Laux, S. E., M. V. Fischetti, and D. J. Frank. "Monte Carlo Analysis of Semiconductor Devices: The DAMOCLES Program." *IBM Journal of Research and Development* 34, no. 4 (Jul. 1990): 466-494.

Can also be found in Fischetti, M. V., and S. E. Laux. "Monte Carlo Simulation of Submicron Si MOSFETs." In *Simulation of Semiconductor Devices and Processes*. Vol. 3.: Proceedings of the Third International Conference on Simulation of Semiconductor Devices and Processes, held at the University of Bologna, Bologna, Italy, on September 26th-28th, 1988. Edited by G. Baccarani and M. Rudan. Bologna, Italy: Technoprint, 1988, pp. 349-368.

Close to edges:

$$g_c(E) \propto \sqrt{E - E_c} \qquad E \ge E_c$$

$$g_v(E) \propto \sqrt{E_v - E} \qquad E \le E_v$$





Common expressions for DOS:

$$g_c(E) = 4\pi \left(\frac{2m_{de}^*}{h^2}\right)^{3/2} \sqrt{E - E_c} \qquad E \ge E_c$$

$$g_v(E) = 4\pi \left(\frac{2m_{dh}^*}{h^2}\right)^{3/2} \sqrt{E_v - E} \qquad E \le E_v$$

 $m_{de}^* \equiv$ density of states electron effective mass $m_{dh}^* \equiv$ density of states hole effective mass

Key conclusions

- Concept of *(free) electron*: electron in conduction band.
- Concept of *hole*: empty state in valence band.
- Intrinsic semiconductor: ideally pure semiconductor.

$$n_o = p_o = n_i \sim \exp(-\frac{E_g}{2kT})$$

• To first order, for a given semiconductor $n_o p_o$ is a constant that only depends on T:

$$n_o p_o = n_i^2$$

- Equilibrium carrier concentrations can be engineered through shallow dopants \Rightarrow extrinsic semiconductor.
 - n-type semiconductor:

$$n_o \simeq N_D, \qquad p_o \simeq \frac{n_i^2}{N_D}$$

- p-type semiconductor:

$$p_o \simeq N_A, \qquad n_o \simeq \frac{n_i^2}{N_A}$$

- Around edges, conduction and valence bands in semiconductors feature $DOS \sim \sqrt{E}$.
- Order of magnitude of key parameters for Si at 300 K:
 - intrinsic carrier concentration: $n_i \sim 10^{10} \ cm^{-3}$
 - typical doping level range: N_D , $N_A \sim 10^{15} 10^{20} \ cm^{-3}$

Self study

• Charge neutrality