2015, Spring Semester

Energy Engineering (Class 458.624)

Professor

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 \Box C hass t in e : M onday, W ednesday 1100 ~ 12:15

Textbook

- (1) Introduction to Solid State Physics (Charles Kittel)
- (2) Solid State Electronic Devices (Ben G Streetman, Sanjay Kum ar Benerjee)

Chapter 3. Energy Bands and Charge Carriers in Sem iconductors

We are interested in

- (1) How to make different charge distribution: use doping, n+ and p+ type regions in p and n type substrate
- (2) How to make carriers(charges) move(transport) from one bcation to the other in a controlled way (by applying bias gate bias to form a conducting channel, drain bias to let majority carriers move)

Let's try to understand energy bands, doping, Ferm i level, etc., which are fundamental concepts of above issues in solid state electronic devices

Cova lent Bonding

Now we can examine elemental and compound semiconductors.

- Each atom shares bonds with 4 other atoms.
- Silicon bonds are covalent, but compound semiconductors have a mix of ionic and covalent bonds.
 - Depends on separation on periodic table.



DIAMOND CRYSTAL STRUCTURE WITH TETRAHEDRAL BONDING ... EXAMPLES INCLUDE SILICON & GERMANIUM



When silicon atoms COMBINE to form a crystal the s- and p- orbitals HYBRIDIZE to form so-called sp³ ORBITALS that are mixtures of the s- and p-orbitals.



Bands



Figure 3.2

-Figure 32 (left) shows schem at ic coulom bic potential wells of two atoms.

-The composite two-electron wave functions are linear combination of individual atom ic orbitals. Antisymmetric combination is antibonding and symmetric combination is bonding orbital.

-Bonding orbitalhas higher value of wave function (more electron) in between the two nuclei.

-Since electrons in between are attracted by two nuclei, the potential energy of bonding is bwer than ant bonding.

-The number of distinct energy levels (splitted by bonding and ant bonding) depends on the number of atoms brought together. -The bwest and highest energy level correspond to entire bonding and entire ant bonding.

h a solid, <u>m any atom s are brought together, so that the split</u> energy <u>evels</u> from essentially continuous bands of energy.
h silicon, the upper band (conduction band) contains 4N state (no electron at 0 K) and bwer band (valence band) contains 4N state (4N electrons at 0 K). There is a forbidden state, called a band gap, between the two bands.



Bands and Band Gap



- The top band is referred to as the "conduction" band.
 At low temperatures it is mostly empty of electrons.
- The bottom band is referred to as the "valence" band.
 - At low temperatures it is almost entirely filled with electrons.

Metal, Insulator and Sem iconductor

Let's use the band gap to classify these different classes of materials...



M easurem ent of Eg



Band gap energies of selected semiconductors

Semiconductor	Ge	Si	GaAs
Band gap (eV)	0.67	1.12	1.42

- Band gap energy of a sem conductor material can be measured by photon absorption energy.
- The m in in um energy of photons that are absorbed by the sem iconductor (h_v) is the band gap energy (Eg).
- Othermaterials:TD2 (32),ZnO (33),SBN4(5),SD2(9)

Density of States



- The density of states (g(E)) describes the num ber of states per interval of energy at each energy level that are available to be occupied by electrons.
- ie.g(E)dE = num ber of states/cm³ in the energy range between E and E+dE.

Effective M ass



Group	Material	m _n *	m _p *
IV	Si (4K)	1.06	0.59
	Si (300K)	1.09	1.15
	Ge	0.55	0.37
III-V	GaAs	0.067	0.45
	InSb	0.013	0.6
II-VI	ZnO	0.29	1.21
	ZnSe	0.17	1.44

- The electrons in a crystallare not completely free, but instead interact with the periodic potential of the lattice. The interacting force is different in different materials and different directions in one material.
- A particle's effective mass (often denoted m *) is the mass that it seem s to have when responding to forces. (higher interaction ~ heavier effective mass)
- For electrons or holes in a solid, effective mass is usually stated in units of the true mass of the electron m_e ,9.11× 10⁻³¹kg.

$$h/2\pi)^2$$

m *= $\frac{(h/2\pi)^2}{d^2E/dk^2}$

high curvature at CB m in im um and VB m axim um in E-k diagram ~ bw effective m ass

Direct and Indirect

Direct gap versus Indirect gap...



- E-k diagram : A lbwed values of E vs k (wave vector, m om entum of e^- and h^+) can be p btted.
- Since the periodicity of most crystal lattices is different in various directions of electron movem ent, relationship between E and k are plotted as above.
- Direct gap material (like GaAs) has the conduction band minimum and valence band maximum at the samek, while indirect gap material (like Si) has them at different k.
- In the case of indirect gap, the electron should change the direction of movement to move between m in imum and maximum and thereby involves with momentum change in k.
- In direct gap, an electron in CB fails to an empty space of VB and gives off photons (light).
- In indirect gap, the momentum changes are needed and phonon involves, which emits energy change as a heat instead of light.
- Generally, optoelectronic devices, like LED, are made of direct gap materials.

Band Change in A lby

We can tailor the band gap in compound semiconductors

-D ifferent com pound sem conductors have different band structure, which can be tuned by a lbying different materials.

-GaAs and AAs can be a lbyed to make A $LGa_{Hx}As$. -Depending on the AI fraction in a lby the band gap structure changes from indirect gap (AAs) to direct gap (GaAs), as shown in the following diagrams.





Electrons and Holes



-Sem conductors differ from metals and insulators by the fact that they contain an "a most-empty" conduct on band and an "a most-full" valence band (> OK). This also means that we will have to deal with the transport of carriers in both bands. -To facilitate the discussion of the transport in the almost-full valence band of a sem conductor, we will introduce the concept of holes.

-The concepts of holes is introduced in sem iconductors since it is easier to keep track of the m issing electrons in an "almost-full" band, rather than keeping track of the actual electrons in that band.

-Holes are m issing electrons. They behave as particles with the same properties as the electrons would have when occupying the same states except that they carry a positive charge. This definition is illustrated further with next slide, which presents the energy band diagram in the presence of an electric field.

Electric Field

Now put the semiconductor in an electric field...



-(E,k) diagram is a pbt of the total electron energy (potential + kinetic) as a function of the crystaldirection dependent electron wave vector (k,which is proportional to the momentum).

-D ifferent crystaldirection has different E-k diagram -Therefore the bottom of the conduction band (where k=0) corresponds to zero electron velocity or kinetic energy and simply gives the potential energy at that point.(left)

-Energies higher in the band than the minimum k point corresponds to additionalkinetic energy of the electron (potential+kineticE).

-Since the band edge corresponds to the electron potential energy, the variation of the band edge in space is related to the electric field at different points of sem iconductor.

- h the left diagram, electron at location A sees an electric field given by the slope of the band edge (potential energy), and gains kinetic energy (at the expense of potentialE) by moving to point B (less potentialE, more kineticE).

-The sbpe of band edge represents bcale bctric field of each point.

Intrinsic Materials

Intrinsic Material is pure with no additional contaminants...



- At T = 0 K, there is no energy in the system.
 - All of the covalent bonds are satisfied.
 - Valence band is full and conduction band is empty.
- At T > 0 K, thermal energy breaks bonds apart
 - Crystal lattice begins to vibrate and exchange energy with carriers.
 - Electrons leave the valence band to populate the conduction band.

Putting temperature and band gap together to obtain carriers...



- Thermal excitation cause bonds to break
 - At T = 0 K there is no energy to break bonds.
 - Valence band is totally full and conduction band is empty.
 - At room temperature, carriers can be excited across the band gap.
 - This liberates electrons and holes.

But there are more processes at work...



- Generation
 - Break up of a covalent bond to form an electron and a hole.
 - Requires energy from thermal, optical, mechanical or other external sources.
 - Supply of bonds to break is virtually inexhaustible.
 - Atomic density >> # of electrons or # of holes.

Since we are in thermal equilibrium, there must be an opposite process...



- Recombination
 - Formation of a bond by bringing together and electron and a hole.
 - Releases energy in the form of thermal or optical energy.
 - Recombination events require the presence of 1 electron and 1 hole.
 - These events are most likely to occur at the surfaces of semiconductors where the crystal periodicity is broken.
 (Surface recombination ~ important in photovoltaic devices)



 The generation rate must be balanced by the recombination rate.

$$G_0 = R_0 \Rightarrow n_0 p_0 = n_i^2$$
 $n_0 = p_0 \Rightarrow n_0 = p_0 = n_i$

• Important consequence is that for a given semiconductor the *np* product depends only on the temperature.

Now, we learned...

(1) Conduct ion and Valence Band
(2) Band Gap
(3) Electron and Hole, their pair
(4) Band Bending by External Electric Field
(5) Therm al Generation and Other Generations
(6) Recombination, Illuminating and Thermal

Then How Can We ControlLocalCarrier Concentrations? Ex) n+,p+,n and p

By Doping…

Extrinsic Materials

The great strength of semiconductors...

- We can change their properties many orders of magnitude by introducing the proper impurity atoms.
- Which columns add
 - Electrons?
 - Holes? -
- What about impurities?
 - -Doners and Acceptors









So, let's review doping of elemental semiconductors ...

- Dopants in Silicon
 - Reside on the lattice sites.
 - Group V elements contribute electrons to the conduction band and are called donors.
 - Group III elements contribute holes to the valence band and are called acceptors.
 - These impurities are totally ionized at room temperature.
 - Concentrations range from 1014 cm⁻³ to 10²⁰ cm⁻³.

Low doping (channel) High doping (contact)

Norma

bond

Boron

Hole

atom

In general, we can modify the materials properties with the introduction of immobile impurity atoms...

- We can
 - Selectively create regions of *n* and *p*.
 Needed for CMOS.
 - Modify the conductivity over several orders of magnitude.
 - Manipulate the number of conduction electrons over 5 orders of magnitude.

(From 10¹⁴ to 10²⁰)



Band Diagram of Silicon with Donors and Acceptors



Let's take a look at Silicon with Phosphorus impurity atoms:



Therm a IExcitation of Intrinsic Materials

Putting temperature and band gap together to obtain carriers...



- Thermal excitation cause bonds to break
 - At T = 0 K there is no energy to break bonds.
 - Valence band is totally full and conduction band is empty.
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Therm a IExcitation of Extrinsic Materials

Revisiting the effect of temperature ...



M uch easier therm a IEHP generation with donors and acceptors !!

Term s

Commonly used terms:

- Dopants specific impurity atoms that are added to semiconductors in controlled amounts for the express purpose of increasing either the electron or hole concentrations.
- Intrinsic semiconductor undoped semiconductor; extremely pure semiconductor sample containing an insignificant amount of impurity atoms; a semiconductor whose properties are native to the material.
- Extrinsic semiconductor doped semiconductor; a semiconductor whose properties are controlled by added impurity atoms.
- Donor impurity atom that increases the electron concentration; n-type dopant.
- Acceptor impurity atom that increases the hole concentration; p-type dopant.
- N-type material a donor doped material; a semiconductor containing more electrons than holes.
- P-type material an acceptor doped material; a semiconductor containing more holes than electrons.
- Majority carrier the most abundant carrier in a given semiconductor sample; electrons in ntype and holes in p-type.
- Minority carrier the least abundant carrier in a given semiconductor sample; electrons in ptype and holes in n-type.

Now, we learned...

(1) Conduction and Valence Band, Band Gap
(2) Electron and Hole, their pair
(3) Band Bending by External Electric Field
(4) Therm al Generation and Other Generations
(5) Recombination, Illuminating and Therm al
(6) Control of Local and/or Overall Concentrations of Electrons and Holes by Doping

Then How Can We Express The Amount of Specific Carrier (Either Electron or Hole) in Specific Region? Ex) n-type and p-type Si have different amount of carriers. How can we tell the difference between these two?

We can use the Ferm iLevel to express this...

Ferm iLevel

 The Fermi function tells us the probability of how many of the existing states at any given energy will be filled with an electron.



What about the temperature dependence?

-At tem peratures higher than OK, som e probability exists for states above the Ferm i level to be filled. - h applying Ferm iD irac distribution, f(E) is the probability of occupancy of an available state at E. - h intrinsic materials, $f(E_F) = \frac{1}{2}$, since the num ber of electrons and holes are same.

 $-E_F$ is the energy level where $f(E_F) = \frac{1}{2}$.



Visualizing the Fermi level in intrinsic material ...



In intrinsic material:

- h intrinsic material, the concentrations of holes in VB and electrons in CB are same. Therefore the ferm i level E_f lie in the middle of band gap.

-The symmetry of the distribution of empty and filled states about E_f makes the Fermi evel a natural reference point in calculations of electron and hole concentrations.



- In n-type material:
 - The Fermi level now lies closer to the conduction band.
 - There are many more electrons
 - The difference between E_f and E_v provides a measure of the strength of the doping.





- In p-type material:
 - The Fermi level now lies closer to the valence band.
 - There are many more holes



- Com pare three cases
 (intrinsic, n and p type) in one charts
- Band diagram ,Density of states,Ferm i-dirac distribution and carrier concentrations for intrinsic, n type and p type materials



Junction under Equilibrium



•The contact potential is the voltage necessary to maintain equilibrium at the junction.

Since there should be no current flowing under equilibrium, the Fermi level of PN junction without external bias should be flat.

 $\Rightarrow \text{Therefore } E_{cp} > E_{cn} \& E_{vp} > E_{vn} \\\Rightarrow \text{M ore about junctions in the next chapter}$

Tem perature Effect

What is the role of temperature?? (n-type materials)

Temperature defines three distinct regions of conductivity...



So where does the Fermi level lie for a doped semiconductor??

Fermi level positioning in Si at 300 K as a function of the doping concentration...



i) At higher doping concentration, E_f approaches $E_c(CB)$ or $E_v(VB)$. ii) At higher temperature, therm alcontribution to electron hole pairs becomes higher, which leads to more intrinsic property. (N_A and N_D is acceptor and doner concentration)

Carrier Scattering

-Three major carrier transport:

i) Random thermalmotion, ii) Drift and iii) D iffusion

Carriers are not sitting, what are they doing?

- The carriers are in constant motion!
 - Thermal motion of carriers may be viewed as a random walk.
 - The carriers are interacting with many different things:
 - Lattice vibrations Increases with temperature
 - Other electrons Increases with carrier concentrations
 - Impurities Increases with doping concentrations



So they move quickly, so what?

Let's see how far they go before they scatter ...

Define the characteristic time between collisions:

Define the characteristic length of $\lambda \equiv v_{th} \tau_c$ thermal motion (mean free path): (in meters)

Plug in numbers characteristic of silicon at room temperature:

$$\tau_c \approx 10^{-14} \sim 10^{-13} s$$

$$v_{th} \approx 10^5 \frac{m}{s}$$

$$\longrightarrow \lambda \approx 1 - 10 nm$$
Carriers scatter many times in a typical device!!





$$\mathcal{T}_c$$
 (in seconds)

Drift of Carriers

We want controlled motion of carriers rather than random motion in our device.

Net current in any direction is zero! So let's **apply an electric field** to our semiconductor...



With this information, we can define the drift current ...



We want to define a current, or charge per unit time crossing of observation orientated normal to the direction of current flow.



In portant equations from carrier drift ($<v>=\mu E$, by definition)

Drift current density form of *Ohm's Law* Conduct vity and resist vity

$$\mathbf{J}^{\text{drift}} = \mathbf{J}_{n}^{\text{drift}} + \mathbf{J}_{p}^{\text{drift}} = \mathbf{q}(\mathbf{n}\mu_{n} + \mathbf{p}\mu_{p})\mathbf{E} \qquad \mathbf{J} = \boldsymbol{\sigma}\mathbf{E} = \frac{E}{\rho} \qquad \boldsymbol{\sigma} = \frac{1}{\rho} = \mathbf{q}(\mathbf{n}\mu_{n} + \mathbf{p}\mu_{p})$$

Resistivity

Resistivity - reverse of conductivity

• In n-type semiconductor:

$$o_{\mathbf{n}} \approx \frac{1}{\mathbf{qN}_{\mathbf{d}}\mu_{\mathbf{n}}}$$

• In p-type semiconductor:





Carrier M obility

And from the definition of the current, we can define the mobility ...

Using the definitions for the hole and electron drift currents:

$$J_{n}^{drift} = -qn \langle v_{dn} \rangle = qn\mu_{n}E$$
$$J_{p}^{drift} = qp \langle v_{dp} \rangle = qp\mu_{p}E$$

The electron and hole mobility then becomes:



What can we say about the **mobility** in general?

•Refers to the ease with which carriers move through a host crystal.

Scattering and M obility





Figure 3.23

Variation of mobility with total doping impurity concentration $(N_a + N_d)$ for Ge, Si, and GaAs at 300 K.

Two main competing scattering mechanisms of drifting carriers



D iffus ion of Carriers

 Carriers in a sem iconductor diffuse in a carrier gradient by random thermal motion and scattering from the lattice and impurities, from high concentration to by concentration.

Cf) Drift: driving force - electric field

D if fus ion: driving force - concentration difference

 Example: A pulse of excess electrons injected at x=0 at time t=0 will spread out in time as shown in Fig. 4.12.







Flux = number of particles crossing a unit area per unit time [cm⁻² • s⁻¹]

For Electrons:

$$\mathbf{F}_{n} = -\mathbf{D}_{n} \frac{\mathrm{d}\mathbf{n}}{\mathrm{d}\mathbf{x}}$$

For Holes:

$$\mathbf{F}_{\mathbf{p}} = -\mathbf{D}_{\mathbf{p}} \frac{\mathbf{d}\mathbf{p}}{\mathbf{d}\mathbf{x}}$$

Diffusion current density =charge × carrier flux

$$J_n^{diff} = qD_n \frac{dn}{dx}$$
$$J_p^{diff} = -qD_p \frac{dp}{dx}$$

- If an electric field is present in addition to the carrier gradient, the current densities will each have a drift component and a diffusion component.
- Therefore the total current density is as follows:

$$\begin{aligned} \mathbf{J}_{n} &= \mathbf{J}_{n}^{drift} + \mathbf{J}_{n}^{diff} = \mathbf{q}\mathbf{n}\mu_{n}\mathbf{E} + \mathbf{q}\mathbf{D}_{n}\frac{d\mathbf{n}}{d\mathbf{x}} \\ \mathbf{J}_{p} &= \mathbf{J}_{p}^{drift} + \mathbf{J}_{p}^{diff} = \mathbf{q}\mathbf{p}\mu_{p}\mathbf{E} - \mathbf{q}\mathbf{D}_{p}\frac{d\mathbf{p}}{d\mathbf{x}} \\ \mathbf{J}_{total} &= \mathbf{J}_{n} + \mathbf{J}_{p} \end{aligned}$$

- Majority carriers mainly contribute through drift, while minority carriers contribute through diffusion.
- The concentration of majority current can be much larger than minority current, but the concentration gradient of minority current can be significant.
- Therefore diffusion current by minority carriers sometimes is comparable to drift current by majority carriers (ex.D iffusion - diode, Drift - transistor)

- It is important to discuss the influence of electric field on the energies of electrons in the band diagrams.
- Let's assume E field E(x) in the x direction, then the energy band bending will be as shown in the right figure (Fig. 4.15).

 $E(x) = -dV/dx \text{ or } -\Delta V/I$

- From the definition of electric field, E(x) is as follow:



- For non-uniform doping in equilibrium (no net current), the carrier concentration gradient (due to non-uniform doping) make a diffusion current, while a built-in electric field (by uncompensated charges) makes a drift current.
- For both electron and hole components, the net current is zero and thus drift and diffusion current are canceled out.

$$J_n(x) = J_n^{drift}(x) + J_n^{diff}(x) = 0$$

 $\mathscr{E}(x)$

 E_{v}

In Chapter 3 and 4 (Streetman, Solid State Electronic Devices), we have learned fundamental concepts for electronic device (diodes, transistors, circuits) study.



The questions, when we beg ins these chapters, were

- (1) How to make different charge distribution: n and p type regions
- (2) How to make carriers (charges) move(transport) from one bcation to the other in a controlled way (by applying bias or by making carrier concentration gradient)