Chapter 1 Notes

What is a semiconductor?

Semiconductors are that group of materials having electrical conductivities intermediate between metals and insulators.

Conductivity of semiconductors can vary orders of magnitude due to changes in:

- temperature,
- optical or electrical excitation
- impurity content

Elemental semiconductors are found in Group IV of the periodic table.

Compound semiconductors can be formed from the combination of elements from Group IV and/or neighboring groups of the periodic table (III and V, or II and VI, for example).

<u>The key is 4 valence electrons.</u>

What are they used for?

Germanium – widely used in the early days of diodes and transistors, has good use in very low noise applications today.

Silicon – the mainstream elemental semiconductor used today for rectifiers, transistors and integrated circuits.

Compound Semiconductors – widely used in high speed applications and in applications involving the emission and absorption of light.

- Binary (two elements) such as GaP, GaN, GaAs are common LEDs
- Ternary (three elements) such as GaAsP and quaternary (four elements) such as InGaAsP are "designer semiconductors", fabricated and tuned for particular properties.
- II-VI compounds like ZnS are used for fluorescent coatings in TV screens
- IR and nuclear radiation detectors are commonly Si or GE
- Visible light detectors are typically InSb, CdSe, PbTe or HgCdTe
- Gunn diodes (microwave device) are GaAs or InP
- Semiconductor Lasers are GaAs or AlGaAs

The Energy Band Gap is a primary characteristic distinction between semiconductors.

The band gap determines the wavelength of light that can be emitted or absorbed by a semiconductor, and impacts device switching (speed) and noise characteristics as well. We will study this in detail in chapter 3.

The "width" of the band gap is measured in electron volts (eV). GaAs has a band gap of about 1.43 eV, corresponding to a light wavelength in the near infrared. GaP has a band gap of about 2.3 eV, allowing it to emit green light. The good news is that there is a wide

range of available band gaps from which to construct LEDs, lasers and other absorption and emission devices (see Appendix III).

We can adjust the electronic and optical qualities of semiconductor materials by carefully controlling the type and amount of impurities, called *dopants*, in the materials.

Understanding how a small change (a part per million) in impurity concentration can radically alter electronic properties requires that we know a little about the crystal structure of semiconductor bulk materials.

Periodic Structures, Planes and Directions

The periodic arrangement of atoms is the distinguishing physical characteristic of a crystal.

One point of a pure crystal appears exactly the same as any other equivalent point.

Other solid structures are amorphous and polycrystalline.

Discuss Figure 6-33

- Lattice – spacial array of points (atoms)
- Basis – an atom or atoms at each lattice point, comprising the crystal
- Cell – a regularly repeated volume of the lattice
- Primitive Cell – the smallest regularly repeated volume of the lattice
- Primitive Vectors – vectors connecting adjacent vertices of the primitive cell
- Unit Cell – a conveniently constructed regularly repeating volume of the lattice
- Basis Vectors – vectors defining the unit cell
- Lattice constant – the basis vector of a cubic unit cell.

Unit cell dimensions determine, among other things, the following:

- Distance between neighbor and next neighbor atoms, from which binding forces are determined
- The fraction of the unit cell volume filled by its atoms, from which density of a solid is derived
- Allowable energies of electrons that can participate in conduction

Simple Cubic (sc), Body Centered Cubic (bcc) and Face Centered Cubic (fcc)

Simple Cubic – six sides, eight corners with an atom at each. Each atom is shared by eight adjacent unit cells, therefore only $1/8^{th}$ of each corner atom "belongs" to the unit cell. The number of atoms per cell is 8 times $1/8^{th}$ = 1 atom per unit cell.

Face Centered Cubic – six sides with an atom centered in each, eight corners with an atom at each. Each face atom is shared by two cells, so only ½ of each face atom belongs to the unit cell. The number of atoms per fcc cell is ½ times 6 plus 1 (corner total) = 4.

Body Centered Cubic – same as Simple Cubic, but with one unshared atom in the center of the unit cell. Total number of atoms per bcc unit cell is 2.

Hard Sphere Approximation:

Presumes the atoms are hard spheres and are tightly packed (touching) in their unit cells. The unit cells are cubic, and thus can be assigned a basis vector, called the lattice constant of ***a*** (the distance between adjacent cell corners)

Example 1-1

Body centered cube – lattice constant is 5Å. Three atoms must touch tangentially through the body diagonal of the cube to accommodate the hard sphere model. Two radii of the corner atoms plus one diameter of the body centered atom must equal the cube diagonal.

Pythagoras says the (cube diagonal)^2 = $a^2 + ((a^2 + a^2)^{1/2})^2 = a^2 + (a\sqrt{2})^2 = 3a^2$

Thus the cube diagonal, composed of 4 atomic radii = $a\sqrt{3}$

So each atom has a radius of $1/4\ a\sqrt{3}$ = 2.165 Å

Packing fraction will be $2*4/3лr^3/a^3 = 2*4/3л(1/4\ a\sqrt{3})^3/a^3$ = 68%

Packing fraction: The volume of the hard sphere atoms of each cell divided by the cell volume. Volume of a cube = (lattice constant)^3

Volume of an atom = $4/3лr^3$

Simple Cubic – the atomic radius will be 1/2a because the atoms are touching. The packing fraction will be $4/3л(1/2a)^3/a^3 = (4/3)(1/8)\ л$ = 52%

Face Centered Cubic – the atomic radius is $1/4a\sqrt{2}$ (figure 1-4), so as above the packing fraction is $4*4/3л\ (1/4a\sqrt{2})^3/a^3$ = 74%

Planes and Directions

Miller Indices are used to denote planes and directions in crystals. The x, y and z directions of the unit cell are resolved in to hkl notations as follows:

1. Determine the x, y and z axis intercepts of the plane of interest in basis vector units.
2. Take reciprocals of these and reduce to the smallest set of integers with the same relationship.
3. This set of numbers is the hkl label of that plane.

Figure 1-5

1. x, y and z intercepts are 2, 4 and 1 respectively.
2. Reciprocals of above are ½, ¼, and 1, for which the smallest integer representation is 214 (multiply all by 4).
3. The plane in figure 1-5 should be labeled (214).

Miller indices are also used to describe the distance and angles between planes as explained on page 9 of the text.

Diamond

Diamond is an important semiconductor crystal structure. It has a basis of two atoms on an fcc lattice. Si, Ge and C all have diamond structures. Compound semiconductors often are a diamond lattice also, but with alternating atoms. This is known as a ***zinc-blende*** structure. Some II-VI compounds are a zinc-blende variant known as ***wurtzite***.

The structure can be thought of as fcc with an extra atom located a/4 + b/4 + c/4 from each fcc atom.

Diamond unit cells have the 4 fcc atoms plus 4 more 'extras'. Interestingly the packing fraction is quite a bit less than either fcc or bcc (homework).

Czochralski

A common method of growing single crystal Si using a single rotating seed to extract a single crystal boule of Silicon from a melt.

Doping

As materials solidify, certain physical constraints determine the distribution of impurities in the solid versus that of the liquid. The quantity identifying this property is called the ***distribution coefficient***.

$$k_d = \frac{C_S}{C_L}$$

This is affected by the temperature at the liquid/solid interface and by the growth rate of the solid crystal. Knowing the melt concentration of impurities and the growth parameters allows prediction of the impurity concentration of the solid crystal.

Example 1-4

What melt concentration is needed to yield a crystal with 10^{16} phosphorous atoms/cm^3 if $k_d = 0.35$?

From above, $C_L = C_S / k_d$, or $10^{16}/0.35 = 2.86*10^{16}$ P atoms/cm^3

How much phosphorous would be needed to dope 5 kg of silicon to 10^{16} atoms/cm^3?

Si density (from Appendix III) is 2.33 grams/ cm^3. Therefore 5 kg of silicon is 2146 cm^3.

This means we need $2.86*10^{16}$ P atoms/cm^3 times 2146 cm^3 or $6.14*10^{19}$ phosphorous atoms, or ($6.14*10^{19}$atoms * 31 g/mole)/$6.02 * 10^{23}$ atoms/mole = $3.16 * 10^{-3}$ grams of phosphorous.