Intro to Electronic Properties



Monday, Oct. 20, 2003

MATS275: INTRODUCTION TO MATERIALS SCIENCE

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- · Energy Bands
- · Fermi-Dirac Function
- Classes of Materials

Outline of Next Few Lectures

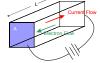
- I. Phenomenological Introduction (Schaffer)
- II. Intro to Quantum Mechanics (Hummel)
- III. Reciprocal Space / Electrons In A Crystal (Hummel)
- IV. Semiconductors (Schaffer / Hummel)
- V. Semiconductor Devices (Schaffer / Hummel)

What Do We Mean by Electrical Properties?

- · Response of a material to an external electric field
- Once again the factors influencing the electrical properties are:
 - chemical bonding
 - number of electrons per atom
 - degree of crystallinity
 - defect density
 - microstructure
 - temperature
 - macroscopic sample dimensions
- · Sound familiar?

Conduction

- Ho do free electrons, move?
- OHM'S LAW



 $\label{eq:V} \mathbf{V} = \mathbf{I} \mathbf{R}$ or more appropriately...

$$\vec{J} = \sigma \vec{E}$$

 σ is conductivity (1/\$\Omega\$-m) $\rho = \frac{1}{\sigma}$



Conductivity (25 orders of magnitude!!!)

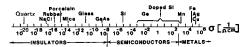


Figure 7.1. Room-temperature conductivity of various materials. (Superconductors, having conductivities of many orders of magnitude larger than copper, near 0 K, are not shown. The conductivity of semiconductors varies substantially with temperature and purity 11 is customary in engineering to use the centimeter as unit of length rather than the meter. We follow this practice.

From R.E. Hummel, Electronic Properties of Materials, 2nd. Ed., Springer-Verlag, 76 (1993)

Applying a Field

• If I apply a field to a conductor:

$$\vec{F} = m\vec{a}$$

$$\vec{F} = m^* \frac{d\vec{v}}{dt} = \frac{d}{dt}\vec{p} = -e\vec{E}$$

• Every $\boldsymbol{\tau}$ seconds, an electron will scatter:

$$\begin{aligned} &-eE\tau = m^*\Delta v & Mobility \\ &-\frac{e\tau}{m^*}E = v_{drift} & \end{aligned}$$

$$\mu_e = \frac{-e\tau}{m^*}$$

Electrons Drifting in an Electric Field

 Classical equation of an electron drifting under the influence of an electric field, with a friction force opposing the field

$$m\frac{dv}{dt} = eE - \gamma v$$

· Solution:

$$v = a[1 - exp(-bt)] \implies v = v_f \left[1 - exp\left(-\frac{eE}{mv_f}t\right)\right]$$

· Drift Velocity:

$$\tau = \frac{mv_f}{eE} \implies v_f = \frac{\tau eE}{m}$$

Mobility and Conductivity

 If the current density is just the number of carriers times the charge times their drift velocity, then...

velocity, then...
$$\vec{J} = \sigma \vec{E} \qquad \frac{-e\tau}{m} E = v_f$$

$$N_f v_f e = \frac{N_f e^2 \tau}{m} E$$

$$\frac{1}{\rho} = \sigma = \frac{ne^2 \tau}{m^*} = ne\mu$$

Mobility like Diffusion Constant

- · Charge Carriers: Ions and electrons
 - lons: move through lattice by diffusion
 - Electrons: Move through lattice relatively unimpeded due to their small size

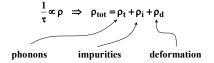
Electrons in Cu

 The conductivity of Cu at 300 K is 5.88 x 10⁵ ohmcm. What is the scattering time?

$$\begin{split} \sigma &= \frac{ne^2\tau}{m^*} \\ \tau &= \frac{m^*\sigma}{ne^2} = \frac{\left(9.11\times10^{-31}\,\mathrm{kg}\right)\!\left(5.88\times10^7\,\Omega\cdot\mathrm{m}\right)}{\left(10^{29}\,\mathrm{m}^{-3}\right)\!\left(1.602\times10^{-19}\,\mathrm{C}\right)^2} \\ \tau &= 2.08\times10^{-14}\,\mathrm{s} \end{split}$$

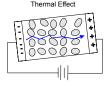
Adding Resistivities

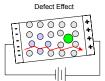
 1/t can be thought of as a rate. The total rate at which electrons are scattered will be the sum of the rates due to different causes:



Mathiessen's Rule

Temperature and Defects--Lower Mobility





Dependence on Impurities

• Note that it is quite linear over a certain range:

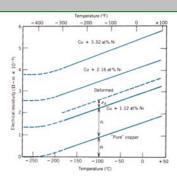
$$\rho_t = \rho_0 + \alpha T$$

· Varies due to impurities:

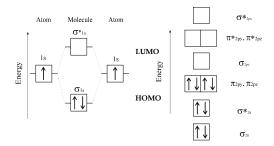
$$\rho_i = Ac_i(1-c_i)$$

• Increased by deformation.

Resistivities

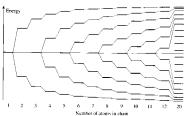


Bonding in Molecules



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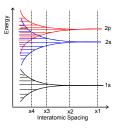
Energy Bands from MO Diagrams



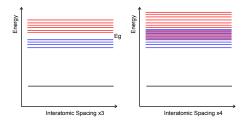
I 2 3 4 5 6 7 8 9 10 11 12 20 Number of atoms in chain

Fig. B.2. The energy levels of A atoms be a chain on the assumption that only rearest-neighbour interactions controlled to bonding. (The Huckel approximation has been used for the Leculation). Note how the density of energy levels in the band increases but that the width remains finite.

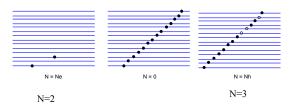
Energy Bands



Band Gap vs. Overlapping Bands

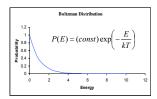


Carrier concentration



It's All Just Statistical

• Macroscopic things (molecules, dust, trucks) can be described with Boltzmann Statistics.



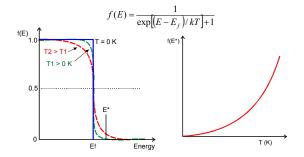
Fermi-Dirac Statistics

 Electrons obey Fermi-Dirac statistics according to the following relationship:

$$f(E) = \frac{1}{\exp[(E - E_f)/kT] + 1}$$

 where E is the energy level in question, E_f is the Fermi energy, and k is Boltzmann's constant

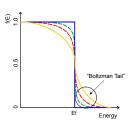
Fermi-Dirac Function



Boltzmann vs. Fermi-Dirac

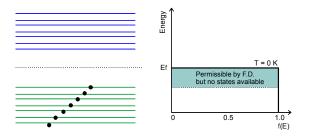
 At very large energies (E >> Ef), we get the Boltzmann distribution

$$f(E) = P(E)$$



How do electrons fill in a band?

Band Filling in a Gap Material at 0 K



Band Filling in a Gap Material above 0 K | Electron in | C.B. | Hole in V.B. | T2 > T1 | T1 > 0 K | Electron in | T2 > T1

Remember that 25 Orders of Magnitude?

How do we classify materials?

Conductor

Semiconductor

Insulator

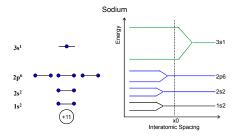
Ev

Ec

Ec

Ec

Conductors--Partially Filled Band



Conductors--Extended Band

Overlapping bands called an extended band

 3s²

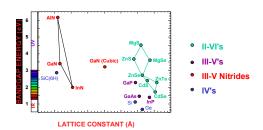
 2p⁶
 2s²
 1s²
 1s²

 Overlapping bands
 Magnesium
 3p0
 3sp0
 2p6
 2sp6
 1s2
 Interatonic Spacing

Semiconductors

- Generally covalent solids such as Si, Ge, GaAs (this is due to hybridization of the s and p orbitals which yields a tetrahedrally bonded solid) This results in a FCC or zinc-blende crystal structure
- Most covalent solids are either semiconductors or insulators because of this.
- Called Group IV, III-V, II-VI
- In addition, most ionic solids are band gap solids which are either an insulator or a semiconductor

Band Gap Energies



Insulators

- Generally metal oxides
- · Silicate ceramics
- · Organic polymers
- All have large band gaps

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