Physics 390 Winter 2007

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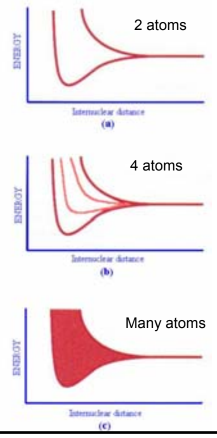
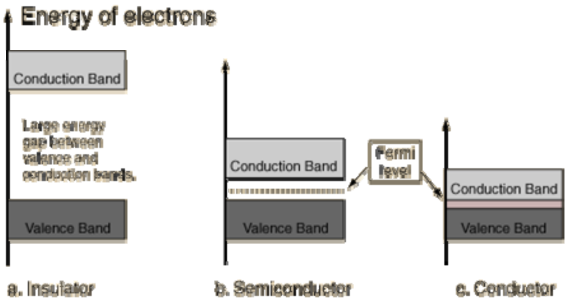
3/15/06

Band theory of solids

- Electronic states of atoms are 'split' by close neighbors
- Many neighbors in a solid create a 'band' of electron energies
- Electric and thermal behavior determined by band filling



Basic effect on electrical properties



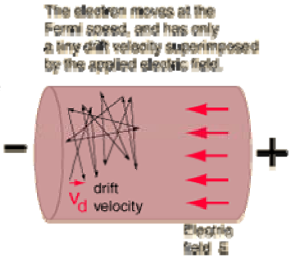
Like Ca (filled 4s) Like Si (details to come…) Like Na (half-filled 3s)

Metals: the electron gas

- In an unfilled band electrons are essentially free
- Electrons move at the "Fermi speed"

$$v_F = \sqrt{\frac{2E_F}{m_e}}$$

- E field imposes small 'drift velocity' on top…



Metals: conductivity

Force is charge*field. $\rightarrow$ $F = -q_e E$

Acc. is force/mass $\rightarrow$ $a = \frac{-q_e E}{m_e}$

Mean velocity (between collisions) depends on τ (collision time) $\rightarrow$ $v \approx \frac{-q_e E \tau}{m_e}$

Current density and conductivity $\rightarrow$ $j = \frac{-n_e q_e E \tau}{m_e} = \sigma E$

Conductivity depends on density and τ $\rightarrow$ $\sigma = \frac{-n_e q_e \tau}{m_e}$

Metals: time to collision

- Electrons move at roughly v_F
- Travel an average distance d_{MFP} = mean free path
- Time between collisions is

$$\tau = \frac{d_{MFP}}{v_F}$$

- Now conductivity is

$$\sigma = \frac{-n_e q_e d_{MFP}}{m_e v_F}$$

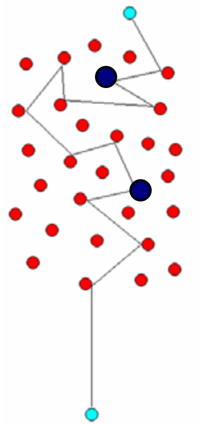
$$d_{MFP} = \frac{\sigma m_e v_F}{-n_e q_e}$$

- Measure σ allows you to find d_{MFP}, which is often large (100x atomic spacing!)

Electrons are rather free!

Metals: mean free path

- Can be strongly affected by impurities
- Is also affected by temperature: if lattice is moving around it's easier to hit one…
- Electrical conductivity may be very sensitive to impurities



Metals: Heat Capacity and Thermal Conductivity

of states at each energy

Heat capacity can be determined. Here g(E) is constant…

$$N_e E_{mean} = \int E p_{FD}(E)\, dE$$

No analytic solution, but approximately

$$E(T) = E(0)\left[1 + \frac{5\pi^2}{12}\left(\frac{kT}{E_F}\right)^2\right]$$

$$\frac{dE}{dT} = C = \frac{5\pi^2 k}{6}\left(\frac{E(0)}{E_F}\right)\boxed{\left(\frac{kT}{E_F}\right)}$$

How much does energy change with temperature?

Electrons contribute to both thermal and electrical conductivity

Ratio of thermal to electrical is the same for all metals

$$\frac{K}{\sigma} = \left(\frac{\pi^2 k^2}{3e^2}\right)T$$

Weidemann-Franz Law

Magnetism in materials

- The basics: what happens when you put a material in a magnetic field?
- Three possible outcomes:
  - Diamagnetism: weak opposition to B field
  - Paramagnetism: weak increase in B field
  - Ferromagnetism: much larger effect
- Applied magnetic field is altered within the material
- $B_{inside} = B_0 + \mu_0 M$
- $M = \mu_{total} / V$
- This is a like a change in magnetic permeability: $\mu = K_m \mu_0$, replace μ_0 in Ampere's law etc.
- K_m = relative permeability which can be > or < 1
- $\chi_m = K_m - 1$: susceptibility

Diamagnetism

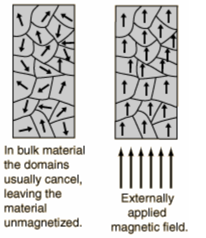
- Orbiting electrons make little current loops
- These loops oppose changes in field like Lenz law: $K_m<1$, $\chi_m<0$
- Materials in which this effect is the only magnetic response are called diamagnetic
- All materials are inherently diamagnetic
- Conductors experience strong diamagnetism with *changing* fields
- Superconductors are perfect diamagnets, *completely* opposing field

Paramagnetism

- Unpaired electron spin lines up with magnetic field imposed from outside
- Effect is lost at high T, where spins get randomized
- M = C (B/T)
- Obviously this doesn't work to very low temperature: it saturates when T goes to zero and all spins are lined up
- Metals don't exhibit this: almost all spins are paired in the conduction band

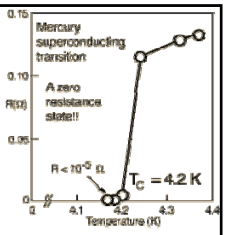
Ferromagnetism

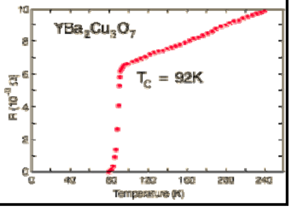
- Some atoms have strong magnetic moments
- At low T, they will align to reduce energy
- This happens within "domains", sometimes small, sometimes large
- Long range order can be induced by external fields to make permanent magnets
- Above the "Curie Temperature", order is lost
- Iron, nickel, cobalt and some of the rare earths (gadolinium, dysprosium)



Superconductivity

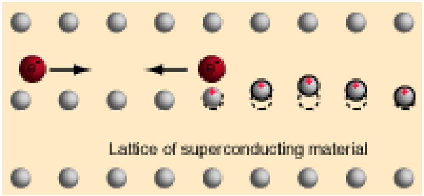
Behavior of resistivity at low temperature:
- Drops to constant for good conductors
- Poorer conductors exhibit "superconductivity"
- Transition is quite sudden and complete





Origins of superconductivity

BCS theory: Cooper pairs
- Electrons pair through interaction with lattice atoms
- One distorts lattice, lattice distortion attracts the other



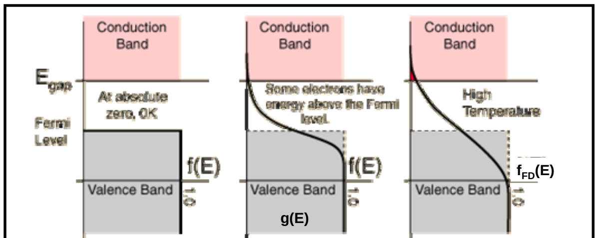
Superconductivity

- Pair of electrons has integer spin: can form Bose-Einstein condensate
- BCS explains SC in simple material, but not high-T_c materials, which remain mysterious

SC applications
- Free current flow, esp. in electromagnets
- Magnets used in imaging (MRI) and levitation (Bullet trains)
- Magnetic exclusion (from Lenz's law)

Semiconductors

- Filled band with a gap in energy before the open 'conduction band'
- Large gap would be an insulator
- Gap is not too large, it's a 'semiconductor'
- At T=0 electrons can't cross and no electrons flow
- At finite T, some electrons get across, leaving "hole" behind



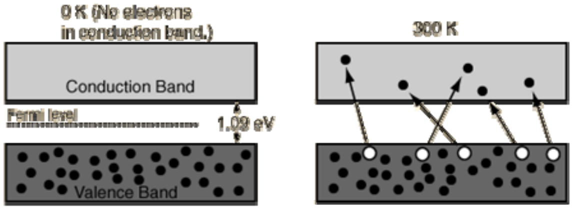
No electrons can be above the valence band at 0K, since none have energy above the Fermi level and there are no available energy states in the band gap.

At high temperatures, some electrons can reach the conduction band and contribute to electric current.

Note: To find the probability that a state will be occupied you must combine the density of states with the Fermi Function

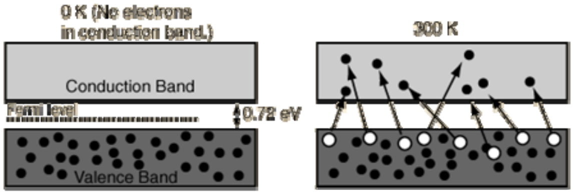
$$p(E)dE = g(E)f_{FD}(E,T)dE$$

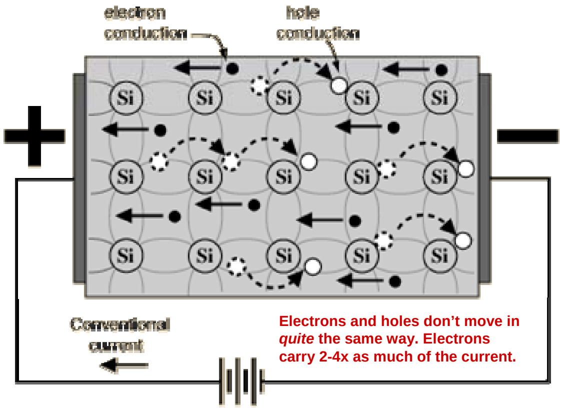
Silicon as a semiconductor



Another important sidelight: the 1.1eV bandgap is equivalent to a photon wavelength of 1.1μm. Shorter wavelength (higher energy) photons, when absorbed, can jump an electron over the gap. The appearance of these electrons can be detected, making silicon a photon detector for optical light **=> Digital CCD cameras**

Germanium as a semiconductor

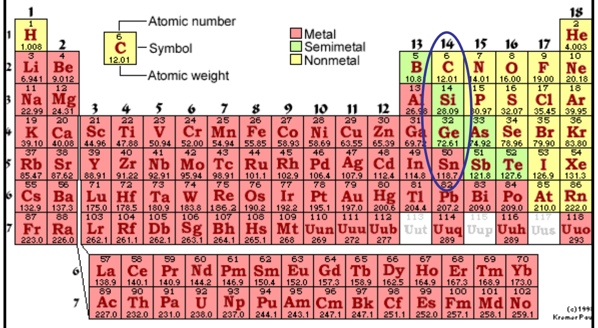




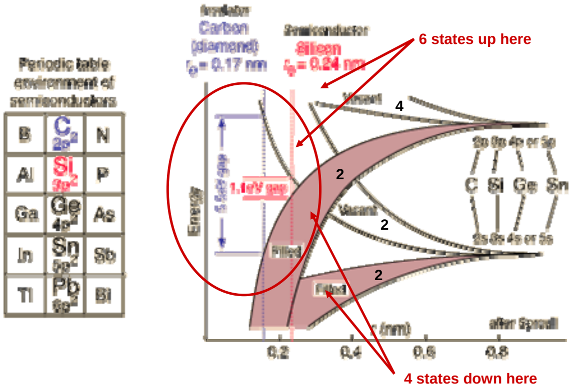
Electrons and holes don't move in *quite* the same way. Electrons carry 2-4x as much of the current.

How to determine where bands lie?

- Recall that in multi-electron atoms states are sometimes not obvious
- In solids, band behaviors are sometimes not obvious, bands can cross
- Good examples include Mg and Si
- Mg is $1s^2 2s^2 2p^6 3s^2$, should be filled and not conduct
- 3p band crosses 3s, allowing conduction states
- Additional interesting cases in the Si column...



All have a filled s shell and 2 electrons in p



6 states up here

4 states down here

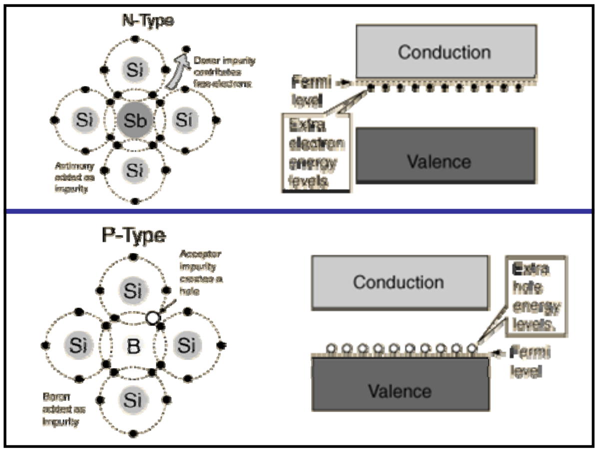
Intrinsic and Impurity Semiconductors

Conductivity:
  - Conductors: all electrons contribute
  - Insulators: None
  - Semiconductors: 10^{-9}

Some homogeneous materials have smallish gaps = intrinsic semicond.

Very sensitive to the presence of impurities

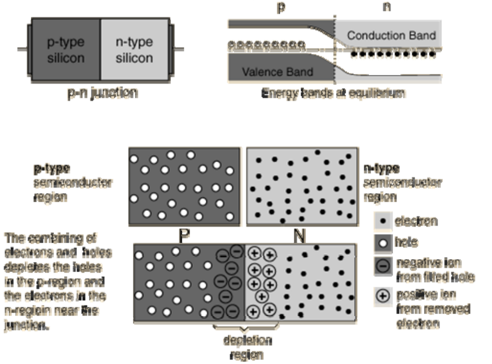
- Impurities can contribute electrons, or use them up, creating holes
- One part in 10^9 can make a big change!
- Dopant with more valence: n-type
- Dopant with fewer valence: p-type



Impurity semiconductors

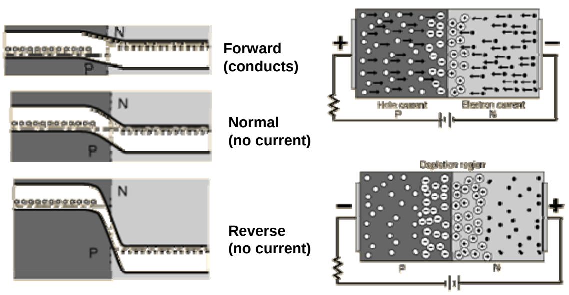
- Such ‘doped’ materials provide a tool-kit for fine tuning the electrical properties of materials
- We can, sometimes, choose the bandgap
- An example: IR detectors
  - IR photons have less energy
  - To detect them, we need a small bandgap
  - $Hg_{(1-x)}Cd_xTe$ can be tuned to alter the band gap (Hg and Cd have the same valence…)

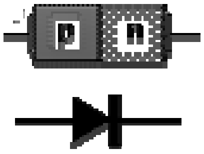
The clever thing: PN junction



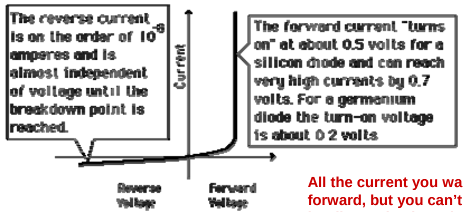
The combining of electrons and holes depletes the holes in the p-region and the electrons in the n-regioin near the junction.

“Biased” PN junction diodes





PN Diodes



The reverse current is on the order of 10^{-8} amperes and is almost independent of voltage until the breakdown point is reached.

The forward current "turns on" at about 0.5 volts for a silicon diode and can reach very high currents by 0.7 volts. For a germanium diode the turn-on voltage is about 0.2 volts

All the current you want goes forward, but you can’t push hardly any backwards. It’s a one-way current valve.