Dr. Gregory W. Clark
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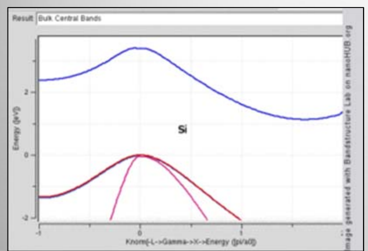
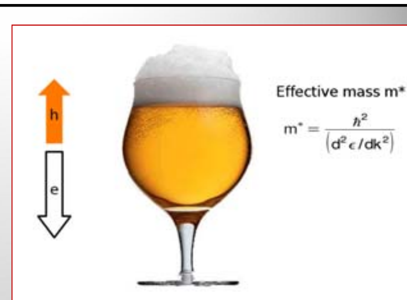
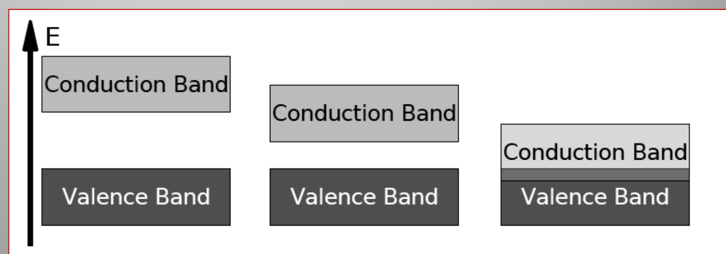




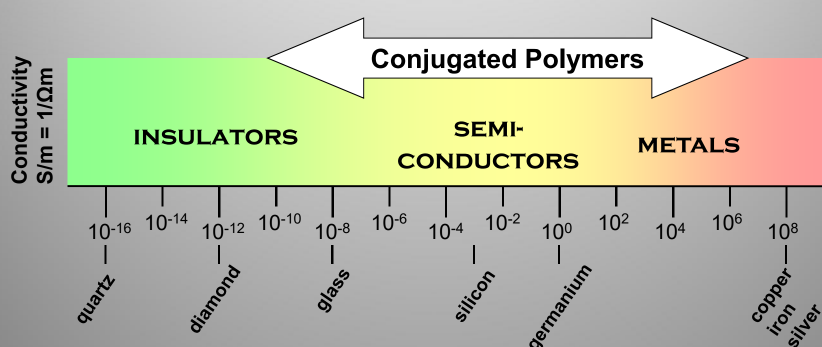


PHYS432

Materials Physics

Electrical conductivity

- Wide range of values!
- Early attempts to model:
  - Drude: free electron gas
  - Sommerfeld: quantum free electron gas



Sommerfeld Theory

(Quantum Free Electron Gas or Free Electron Quantum Model)

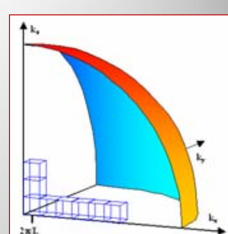
The application of quantum mechanics to statistical mechanics led to modification of Drude's theory to a more apt theory for the many-fermion system.

Fermi-Dirac distribution approaches Maxwell-Boltzmann distribution at large T; most striking differences occur in the vicinity of absolute zero.

Room temperature still low enough for Sommerfeld model to achieve better predictions; most improvements related to thermodynamic phenomena.

Source: Kings College

Quantum Free Electron Gas: Density of available states



- Start with the simple cubic lattice!
- Some definitions:

$$V = L^3 = \text{ volume of unit cell in real space}$$

$$V_G = \left(\frac{2\pi}{L}\right)^3 = \text{ cubic "volume" of unit cell in k-space}$$

$$D_G = \left(\frac{L}{2\pi}\right)^3 = \frac{V}{(2\pi)^3} = \text{density of lattice points in k-space}$$

- Each value of *k* is a different state, but e- can have 2 spin states, so

$$g_k(\vec{k}) = \text{ density of e- states in k-space } = 2D_G = 2\left(\frac{L}{2\pi}\right)^3$$

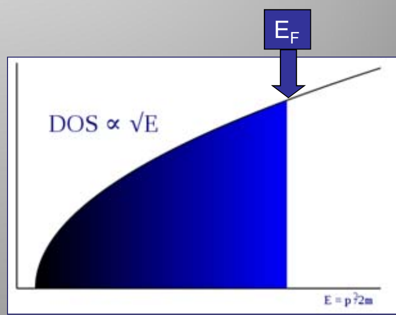
Quantum Free Electron Gas: Density of available states

E_F(eV)	
Na	3.22
Cu	7.00
Ag	5.46
Al	11.58
Au	5.49
Pb	9.38

- For electrons in a SC solid of lattice parameter L, the density of states as a function of energy

$$g(E) = (V/2\pi^2)(2m/\hbar^2)^{3/2} E^{1/2}$$

- The *Pauli Exclusion Principle* requires that we "fill up" this distribution starting at the lowest E



- Energy of the highest state at T=0 is the Fermi energy, E_F:

$$E_F = (\hbar^2/2m)(3\pi^2 N/V)^{2/3} = (\hbar^2/2m)(3\pi^2 n)^{2/3}$$

What about T > 0?

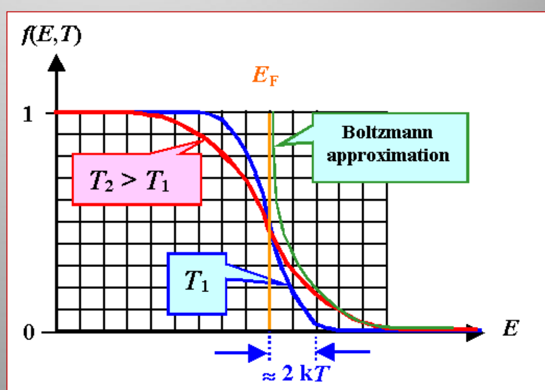
- Fermi-Dirac distribution function:

$$f(E) = \frac{1}{1 + e^{(E-E_F)/k_B T}}$$

where E_F is the Fermi energy and k_B is the Boltzman constant

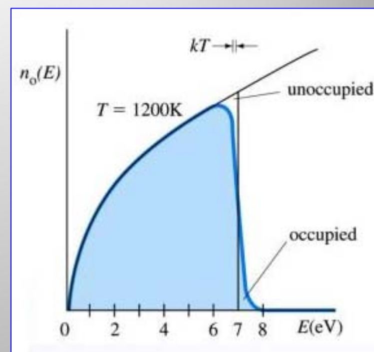
At T = 0,

$$f(E) = \begin{cases} 1, & E < E_F \\ 0, & E > E_F \end{cases}$$



So, the density of *occupied* states is then

$$n_o(E) = DOS = f(E)\, g(E)$$



- The total number of conduction electrons is given by

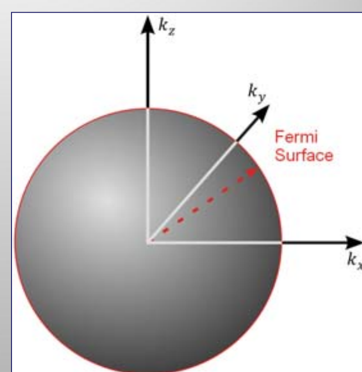
$$N = \int_0^\infty f(E)\, g(E)\, dE$$

* Note that the Fermi energy is a function of temperature; must be chosen to satisfy this integral.

Fermi Surface

- In 3 dimensions, we can define a sphere in k-space of radius

$$k_F = \sqrt{\frac{2mE_F}{\hbar^2}}$$



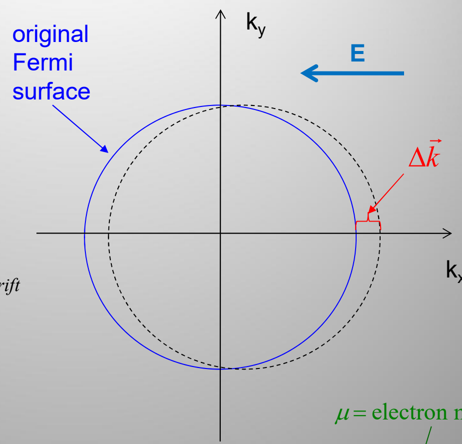
- Electrons having values of k on the surface of this sphere are at the Fermi energy (T = 0)

$$E_F = \frac{4\hbar^2\pi^2}{2mL^2}(n_x^2 + n_y^2 + n_z^2)$$

$$\vec{k} = n_x \frac{2\pi}{L}\hat{i} + n_y \frac{2\pi}{L}\hat{j} + n_z \frac{2\pi}{L}\hat{k}$$

Effect of an electric field

- No field: $\langle \vec{p} \rangle = \langle \hbar \vec{k} \rangle = 0$
  $[\forall \vec{k}\, \exists (-\vec{k})$ to cancel; $\vec{k} = 0]$
- Shift of Fermi sphere
- Center now displaced from origin by $\Delta\vec{k}$
- $\Delta\vec{k} = (1/\hbar)\Delta\vec{p} = (m/\hbar)\vec{v}_{drift}$
  $\left[|\vec{v}_{drift}| \ll |\vec{v}_F| \right]$
- Current flow by electrons with *unmatched* values of k; fits with Ohm's Law

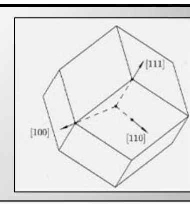


μ = electron mobility

$$J \approx nev_{drift} \approx ne^2\tau E/m = ne\mu E = \sigma E$$

where τ is the ave. time between e- collisions

Band structure – Na (BCC)



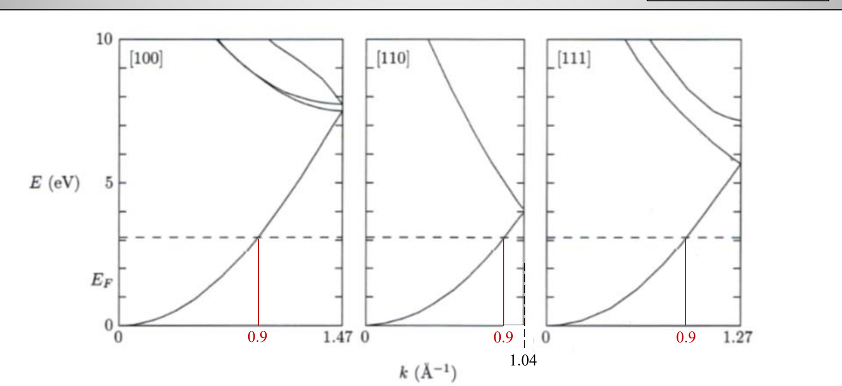
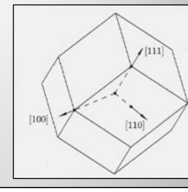
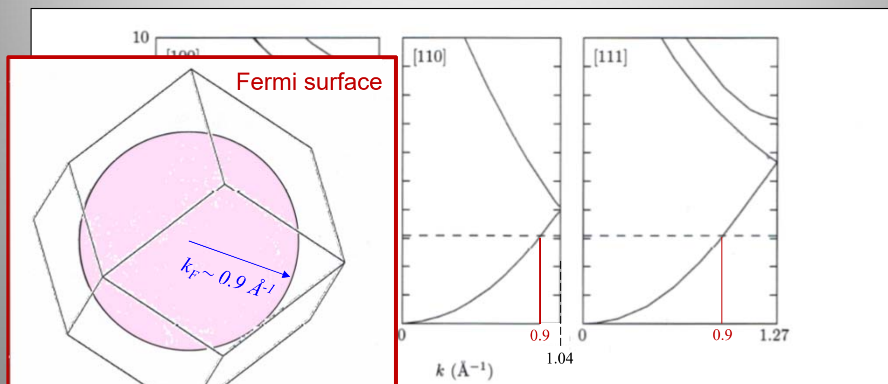


Fig. 8-10. The first Brillouin zone and the energy bands in sodium metal. See D. A. Papaconstantopoulos, *Handbook of the Band Structure of Elemental Solids* (Plenum, New York, 1986)

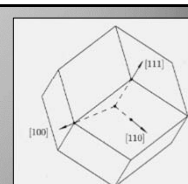
Band structure – Na (BCC)





...ergy bands in sodium metal. See D. A. Papaconstantopoulos, ... *olids* (Plenum, New York, 1986)

Band structure – Ba (BCC)



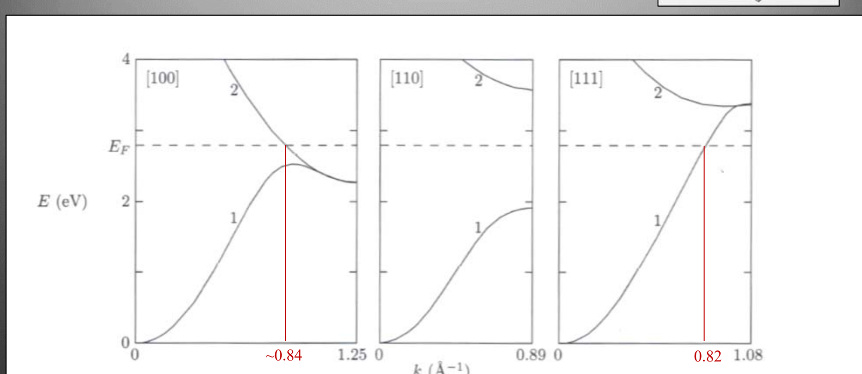
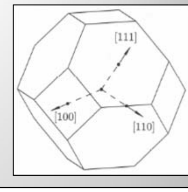


Fig. 8-13. Energy bands in barium metal. The first Brillouin zone is the same as that of sodium, shown in Fig. 8-6. See D. A. Papaconstantopoulos, *Handbook of the Band Structure of Elemental Solids* (Plenum, New York, 1986).

Band structure – Cu (FCC)



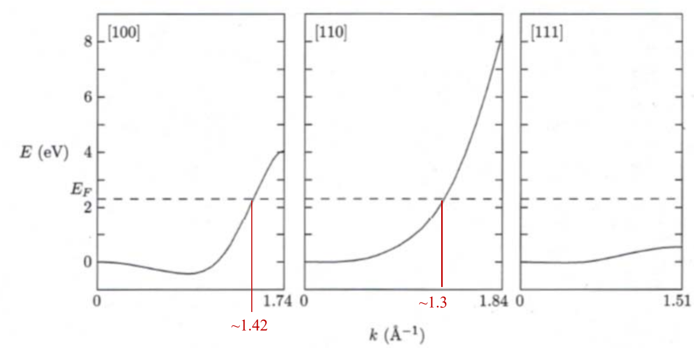
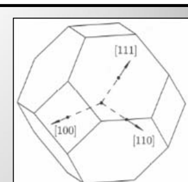
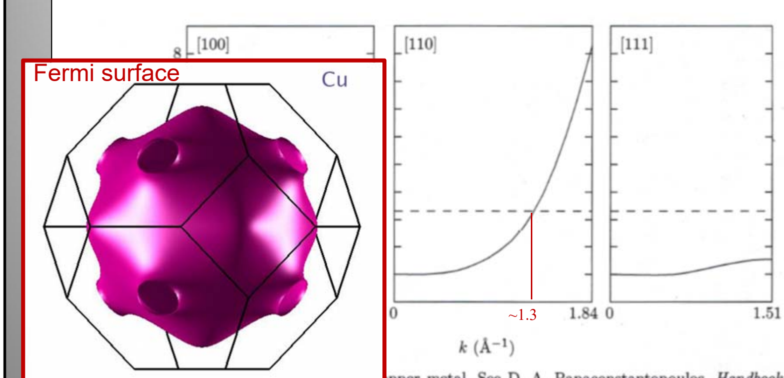


Fig. 8-15. Conduction-electron band in copper metal. See D. A. Papaconstantopoulos, *Handbook of the Band Structure of Elemental Solids* (Plenum, New York, 1986).

Band structure – Cu (FCC)

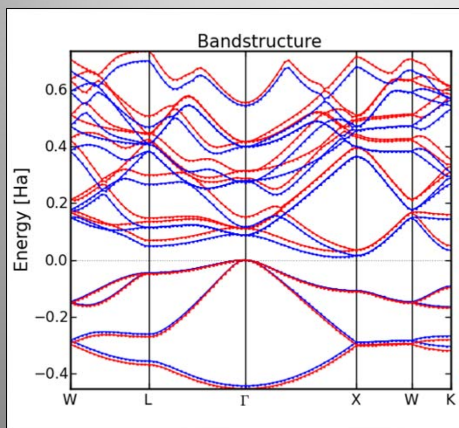


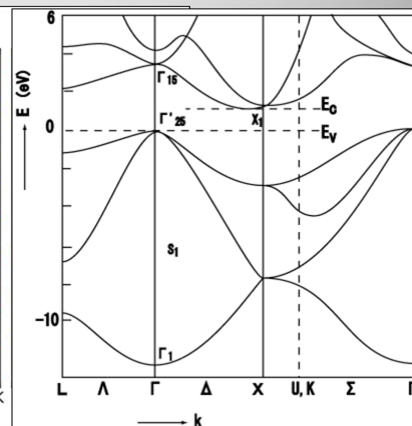


...pper metal. See D. A. Papaconstantopoulos, *Handbook of the Band Structure of Elemental Solids* (Plenum, New York, 1986).

Band structure - Si

A more complicated picture – indirect semiconductor





Successes?

- Free electron gas model explains electrical conductivity reasonably well for some materials (*e.g.*, low carrier concentrations); close to classical result
- Explains classical Hall effect
- Does not completely explain heat capacity, thermal conductivity, thermoelectric effect, magnetic properties, photoelectric effect, *etc.*

Contact Potential:
two unlike metals

- Work function = minimum energy required to remove an e- from a metal
- CPD, = contact potential difference = Δφ, develops across the junction (Metal2 is at higher potential than Metal1)
- Δφ is T dependent (thermocouples)
- *Kelvin method* (a nulling method) can be used to determine work function of unknown metal

CPD
$= \varphi_1 - \varphi_1$

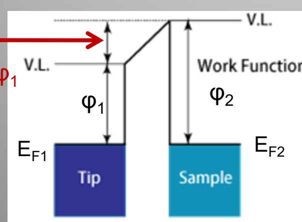
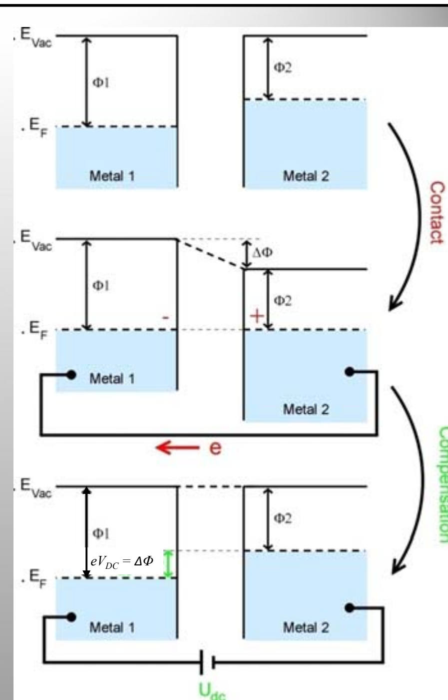
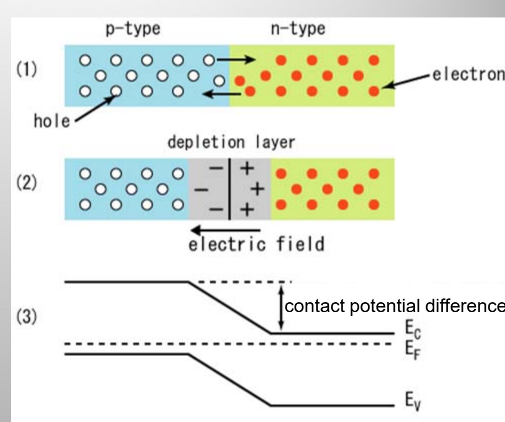


Fig. 1 Band diagram of tip and sample



p-n junction

- Formation of depletion layer & CPD
- Diffusion of majority carriers + recombination creates depletion layer (*depletion of majority carries*)



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