

# Brief Comments on Electrical Properties of Materials

Updated 7 December, 2011

## From a Bulk to Atomistic Description of Electrical Conduction

Classical measurements of electrical properties yield these relationships:

$$\begin{aligned}
 V &= IR && \text{Ohm's Law} \\
 R &= \rho L/A && \rho: \text{electrical resistivity } [\Omega \cdot \text{m}], \text{ intrinsic (no geometric dependence)} \\
 \sigma &= 1/\rho && \sigma: \text{electrical conductivity } [(\Omega \cdot \text{m})^{-1}], \text{ intrinsic}
 \end{aligned}$$

A new understanding of the atomic nature of materials in the early 20<sup>th</sup> century led scientists to describe electrical conductivity in terms of the properties of individual charge carriers.

In metals,

$$\begin{aligned}
 \sigma &= n|e|\mu_e && n: \# \text{ of free (valence) electrons per unit volume available for conduction (1/m}^3\text{)} \\
 & && e: \text{charge of an electron (1.6} \cdot 10^{-19} \text{ C)} \\
 & && \mu_e: \text{electron mobility (m}^2\text{/V}\cdot\text{s)}
 \end{aligned}$$

In semiconductors and insulators,

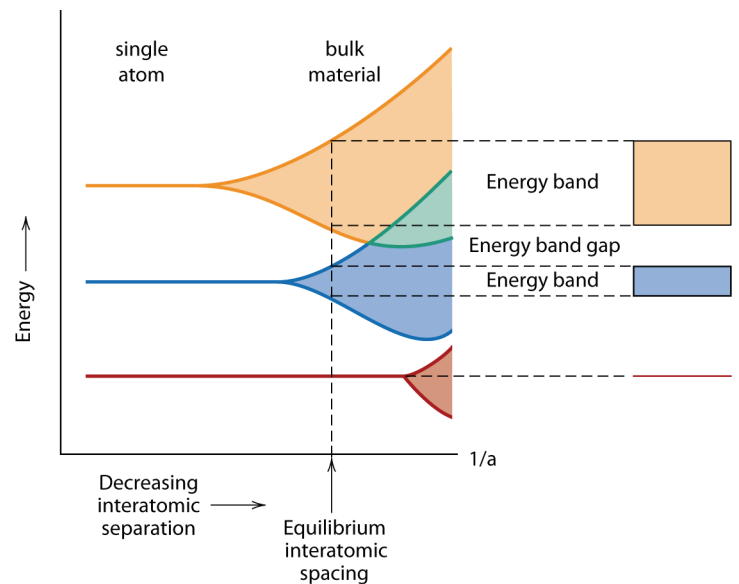
$$\begin{aligned}
 \sigma &= n|e|\mu_e + p|e|\mu_h && p: \# \text{ of holes per unit volume} && \text{hole = empty state below the Fermi} \\
 & && \mu_h: \text{hole mobility} && \text{energy that acts like a charge carrier}
 \end{aligned}$$

$\sigma$  ranges from  $10^{-18}$  to  $10^5$   $(\Omega \cdot \text{m})^{-1}$ . This huge range was explained with the advent of quantum physics.

## From Atoms to Materials

From quantum physics (i.e. by solving Schrödinger's equation), we know that atoms possess discrete energy levels/states (*s, p, d, f*) that its electrons are allowed to reside in.

We can also solve Schrödinger's equation for a bulk (crystalline) material to find the available energy states for that entire system. The system is semi-infinite, involving countless numbers of atoms arranged in the lattice; each atom still contributes its own unique set of discrete energy states. From solving the equation, we find that the energy states from each atom now form a "continuous" band ("continuous" because there are still in fact countless numbers of discrete states, but they are so close together in energy that they can be considered continuous).



The electronic band structure of a material and how electrons reside in it govern the material's electrical properties. ① ②

① *Band structure*

metals

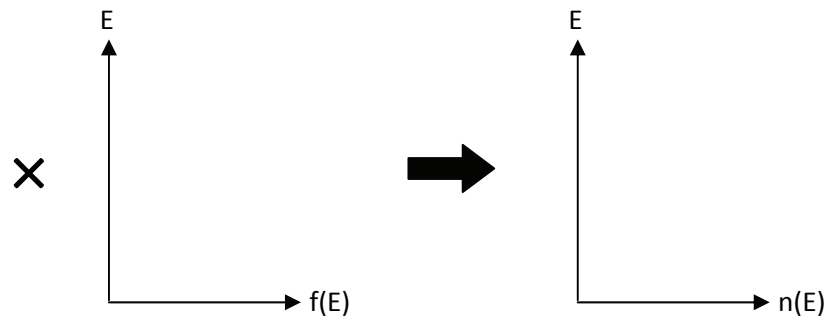
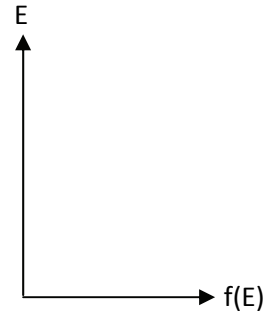
semiconductors

insulators

② *Electron occupation 2a: the Fermi-Dirac distribution*

The Fermi-Dirac distribution describes the probability that an energy state at certain energy would be filled by an electron. Most electrons will tend to fill up lower-energy states first.

The Fermi level or Fermi energy,  $E_F$ , is defined as the energy at which there is a 50% probability that a state at energy  $E_F$  would be filled.



**The availability of empty energy states around  $E_F$  determines a material's electrical conductivity.**

*Electron occupation 2b: relationship to atomic energy levels*

Example	Description	Electronic distribution
Cu [...3d <sup>10</sup> ]4s <sup>1</sup>	Bulk materials made of metallic elements with partially filled valence orbitals have $E_F$ lying within the valence band	
Mg [...2p <sup>6</sup> ]3s <sup>2</sup>	Bulk materials made of metallic elements with filled valence orbitals have overlapping valence and conduction bands	

Si [...2p <sup>6</sup> ]3s <sup>2</sup> 3p <sup>2</sup>  insulators	Bulk materials made of intrinsic semi-conductors or insulators have $E_F$ lying within a bandgap	
---	--	--

## Resistivity in Metals

Review lecture notes.

Resistivity  $\uparrow$  as  $T \uparrow$   
 amount of impurities  $\uparrow$   
 amount of deformation  $\uparrow$

## Semiconductors

### Intrinsic Semiconductors

Intrinsic semiconductors, as mentioned above, have a natural band gap,  $E_g$ , above which electrons must be excited (thermal, EM radiation, etc.) if they are to take part in conduction. The larger the  $E_g$ , the harder it is for electrons to be excited. (ex.:  $E_g^{Si} = 1.1 eV$ ;  $\sigma_{Si} \approx 10^{-4} (\Omega \cdot m)^{-1}$  cf.  $E_g^{Ge} = 0.67 eV$ ;  $\sigma_{Ge} \approx 10^{-2} (\Omega \cdot m)^{-1}$ )  
 Every time an electron is excited above  $E_g$  into the conduction band, a corresponding hole is created in the valence band.

$n_e = \#$  of electrons in the conduction band ( $\#$  of mobile charge carriers)

$$n_e = n_0 \exp\left(-\frac{E_g}{2k_B T}\right) \quad p = n_e \text{ (\# of holes in valence band)}$$

$$n_e \propto 1 / \exp(E_g / T) \text{ (increases exponentially with } T)$$

$$\mu_e \propto 1 / T \text{ (decreases linearly with } T)$$

$$\begin{aligned} \sigma_{\text{intrinsic}} &= n_e |e| \mu_e + p |e| \mu_p \\ &= n_e |e| (\mu_e + \mu_p) \quad n_e = p \text{ for intrinsic semiconductors} \\ &= n_0 |e| (\mu_e + \mu_p) \exp\left(-\frac{E_g}{2k_B T}\right) \end{aligned}$$

$$\sigma_{\text{intrinsic}} \propto 1 / \exp(E_g / T) \text{ [increases exponentially with } T \text{ – the same trend as } n_e!]$$

### Extrinsic (Doped) Semiconductors

See Dr. Wynarsky's handout – it's good!

The primary effect of adding impurities (“doping”) to an intrinsic semiconductors is to introduce loosely-bound charge carriers into the material that can easily be excited into an energy state that allows it take part in conduction. The primary charge carriers for n-type doping are electrons, and holes for p-type doping.

n-type

$$n_e = n_0 \exp\left(-\frac{E_c - E_d}{k_B T}\right)$$

~~$$p = n_0 \exp\left(-\frac{E_g}{2k_B T}\right)$$~~

$$\sigma_{n\text{-type}} = n_e |e| \mu_e + p |e| \mu_h$$

$$\approx \sigma_0 \exp\left(-\frac{E_c - E_d}{2k_B T}\right)$$

p-type

~~$$n_e = n_0 \exp\left(-\frac{E_g}{2k_B T}\right)$$~~

$$p = n_0 \exp\left(-\frac{E_a - E_v}{k_B T}\right)$$

$$\sigma_{p\text{-type}} = n_e |e| \mu_e + p |e| \mu_h$$

$$\approx \sigma_0 \exp\left(-\frac{E_a - E_v}{2k_B T}\right)$$

intrinsic

$$n_e = n_0 \exp\left(-\frac{E_g}{2k_B T}\right)$$

$$p = n_0 \exp\left(-\frac{E_g}{2k_B T}\right)$$

$$\sigma_{\text{intrinsic}} = n_e |e| \mu_e + p |e| \mu_h$$

○ – correction from printed version – so sorry!!!!