Chapter 1: From atoms to solids.

- most materials in nature are made of ~ 30 materials or so and they are comprised of at most 6 elements on average.
- conductivity is measured via resistivity measurements.
- Diamond is a poor conductor (resistivity ~ 10^{22} $\mu\Omega \cdot cm$).
- plastic yield: materials that yield plastic when stressed. They do not break
- Valence electrons determine properties of solids.
- Typical distance between atoms in solids ~ 2-3 Angstrom.
- Crystal shape is determined by manner in which electrons interact.
- Materials can have optical, electronic, thermal, mechanical, magnetic properties?. The question is, how are these properties related to one another?
- Electronic shells can be identified by orbital angular momentum quantum number.
- Core electrons + core => ion

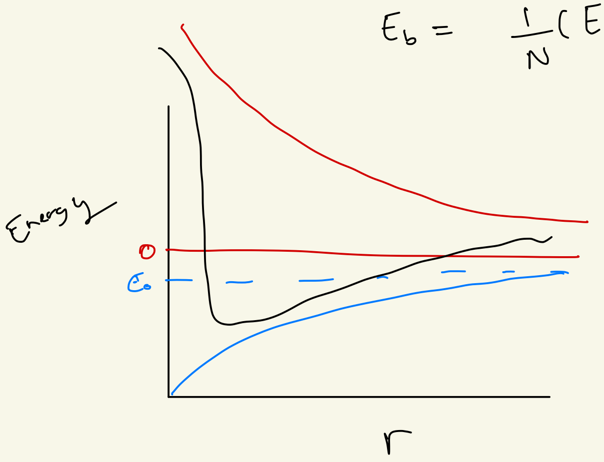
Essence of Metallic (Ionic) bonding:

- In metallic bonding, valence electrons are stripped from core and shared by all cores. The total energy is lower than individual atoms and the difference is the binding energy. Higher binding energy is more stability.
- Optimal structure of solid is when binding energy is lowest.

$$E_b = \frac{1}{N}(E_{tot} - N E_0)$$

E_0 => energy of individual atom).

N => # of atoms.



E_0 => energy of valence elecs bound to cores

A model to understand metallic bonding is Jellium model.

Jellium model :

- No electron interactions
- Ions form a continuous positive background.

Also known as free electron model.

- Wavefunctions in general should respect symmetries the potential. For example uniform and periodic potential lead to wavefunctions that can be described as plane waves.

$$\psi_{\bar{k}}(\bar{r}) = \frac{1}{\sqrt{V}} e^{i\bar{k}\cdot\bar{r}}$$

$\bar{k} \Rightarrow$ wavevector that characterizes $\psi_{\bar{k}}$.

Wave-vectors suffice to characterize single-particle states!

- Wave-vectors take magnitude of 0 up to the fermi momentum which is the wavevector of the most energetic state or the state closest to the Fermi energy

$L^3 \Rightarrow$ volume of box

$$dk_x\, dk_y\, dk_z = \frac{(2\pi)^3}{L_x L_y L_z} \Rightarrow \frac{d\bar{k}}{(2\pi)^3} = \frac{1}{V} \Rightarrow \lim_{V\to\infty} \sum_{\bar{k}} 1 = V \int \frac{d\bar{k}}{(2\pi)^3}$$

$\to$ continuum limit

There is a spin degeneracy thus:

$$2V \sum_{|\bar{k}| < k_F} 1 \rightarrow \frac{2V}{(2\pi)^3} \int_0^{k_f} d^3k \Rightarrow \frac{2V}{(2\pi)^3} \int_0^{k_f}\int_0^{2\pi}\int_0^{\pi} k^2 dk \sin\theta\, d\theta\, d\phi$$

In the free electron model, one obtains the number of one electron states with $|\bar{k}| < k_F$ by integrating over a sphere of radius k_F.

$$\Rightarrow \frac{2V}{(2\pi)^3} \left[\frac{1}{3}k^3\right]_0^{k_F} \left[-\cos\theta\right]_0^{\pi} \left[\phi\right]_0^{2\pi} = \frac{2V}{(2\pi)^3}\cdot\frac{1}{3}k_F^3\,[2]\,[2\pi]$$

$$= \frac{8V\pi k_F^3}{8\pi^3\cdot 3} = \frac{Vk_F^3}{3\pi^2} = N$$

In the free electron model, to find the # of occupied states, we integrate over a sphere of radius k_F. This will yield the # of electrons with $|\bar{k}| \leq k_F$. Let $n = \frac{N}{V}$

$$n = \frac{k_F^3}{3\pi^2} \Rightarrow \text{density of electrons.}$$

$\varepsilon_{\bar{k}} = \frac{\hbar^2 k^2}{2m}$ $\quad k_f = (3\pi^2 n)^{1/3}$ $\quad \varepsilon_{\bar{k}=\bar{k}_F} = \frac{\hbar^2 k_F^2}{2m}$

$$= \frac{\hbar^2}{2m}(3\pi^2 n)^{2/3}$$

We found an expression for the number of occupied states in a free electron model. Occupied states on the ones whos $|\bar{k}| \le k_F$. More energetic elcs will be free.

$$dk_x dk_y dk_z = \frac{(2\pi)^3}{V} \qquad \frac{d^3k}{(2\pi)^3} = \frac{1}{V} \qquad \lim_{V\to\infty} \sum_{\bar{k}}$$

$$V\int \frac{d^3k}{(2\pi)^3} \Rightarrow 2V \sum_{|\bar{k}| \le k_F} \Rightarrow 2V \int_0^{k_F} \frac{d^3k}{(2\pi)^3}$$

$\to$ replace by spherical coords.

$\downarrow$

$k^2 dk \sin\theta \, d\theta \, d\phi$.

$$\lim_{V\to\infty} \sum_{\bar{k}} \Rightarrow V\int \frac{d^3k}{(2\pi)^3} \Rightarrow$$ when you can integ based on Fermi velocity.

In the free electron model, $E_{tot} = E_{kin}$:

$$E_{kin} = \sum_{\bar{k}} \varepsilon_{\bar{k}} = \frac{2V}{(2\pi)^3} \int_0^{k_F} d^3k \, \frac{\hbar^2 k^2}{2m}$$

$$= \frac{2V}{(2\pi)^3} \cdot \frac{\hbar^2}{2m} \int_0^{k_F} k^4 \, dk \int_0^{\pi} \sin\theta \, d\theta \int_0^{2\pi} d\phi$$

$n = \frac{N}{V}$

$V = nN$

$$= \frac{V\hbar^2}{8\pi^3 m} \cdot \frac{1}{5} k_f^5 \cdot 2 \cdot 2\pi = \frac{\hbar^2 V k_F^5}{10\pi^2 m}$$

$$= \frac{\hbar^2 k_f^2}{2m} \cdot \frac{k_f^3 V}{5\pi^2}$$

$\frac{V k_f^3}{3\pi^2} = N$

$V = \frac{3\pi^2 N}{k_f^3}$

$$= \varepsilon_F \cdot \frac{\cancel{k_f^3}}{5\cancel{\pi^2}} \cdot \frac{3\cancel{\pi^2} N}{\cancel{k_f^3}}$$

$$E_{kin} = \frac{3}{5}\varepsilon_F N = E_{tot}$$

$r_s \Rightarrow$ radius of sphere whose volume contains one electron.

$$\frac{4\pi r_s^3}{3} = \frac{V}{N} = n^{-1} = \frac{3\pi^2}{k_f^3}$$

$$k_F^3 = \frac{3\pi^2 \cdot 3}{4\pi r_s^3} = \frac{9\pi}{4} \cdot \frac{1}{r_s^3} \Rightarrow k_F = \left(\frac{9\pi}{4}\right)^{1/3} \cdot \frac{1}{r_s}.$$

Bohr units: Binding energy of ground state of Hydrogen in Bohr model

$a_0 \Rightarrow$ Bohr model.

Proximity of atoms breaks energy degeneracy!

- Induces bonding and anti bonding states. The former are lower in energy than the latter.
  - Bonding states have energy lower than energy of valence states whereas anti bonding has energy higher.