

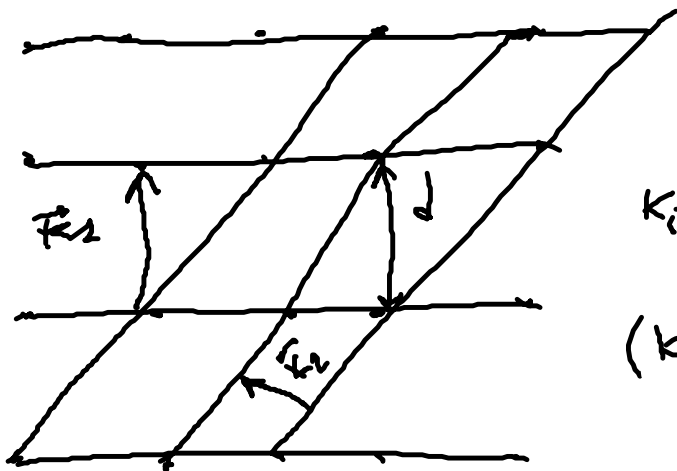
Reminder (Lattice periodicity)

- Bravais lattice
- Wigner-Seitz cell
- Symmetries and crystal systems
(7 crystal systems
and 14 Bravais lattices in 3D)

- Bloch theorem $\Rightarrow \vec{k}$ appears

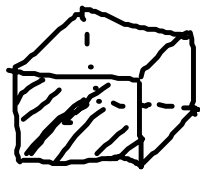
- Reciprocal space and Brillouin zone

Side view of a crystal



$$k_i = \frac{2\pi}{d_i}$$

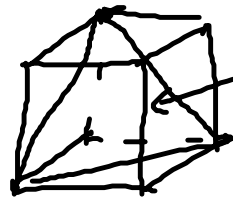
$(k_x, k_y, k_z) \rightarrow$ Miller indices



$\uparrow (100)$

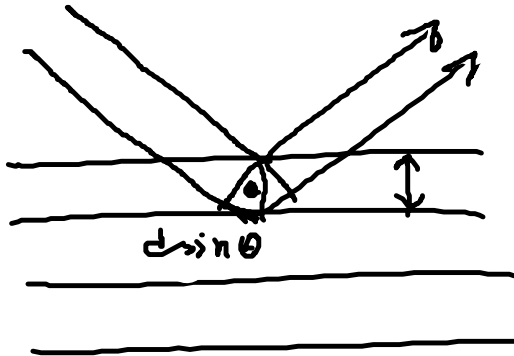


(110)



(111)

Connection to reflection (photons or electrons)



Condition of reflection \Rightarrow Bragg condition

$$2d \sin \theta = m \lambda = m \frac{2\pi}{|\vec{k}|} \quad m \in \mathbb{Z},$$

$\lambda \equiv \text{wavelength}$

$$\Rightarrow \vec{k}^2 = (\vec{k} - \vec{G}_m)^2$$

Chapter 5 Band structure of the electrons

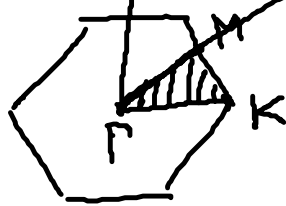
$$\psi_{\vec{k}}(\vec{r}) = \sum_n c_{\vec{G}_n}(\vec{k}) e^{i(\vec{k} - \vec{G}_n) \cdot \vec{r}}$$

$$h_{n,m} = \frac{\hbar^2}{2m} (\vec{k} + \vec{G}_n)^2 \delta_{n,m} + v^{eH}(\vec{G}_n - \vec{G}_m)$$

$$\Rightarrow \epsilon_n(\vec{k})$$

What happens in 2D? $\vec{G}_2 = \frac{2\pi}{a}(0, 2)$

Example:



$$\vec{G}_2 = \frac{2\pi}{a} \left(\frac{\sqrt{3}}{2}, \frac{1}{2} \right)$$

(if all components of $\vec{r}^{stt}(\vec{G}_n)$ are small

$$\Rightarrow \epsilon_n(\vec{k}) = \frac{\hbar^2}{2m} (\vec{k} + \vec{G}_n)^2$$

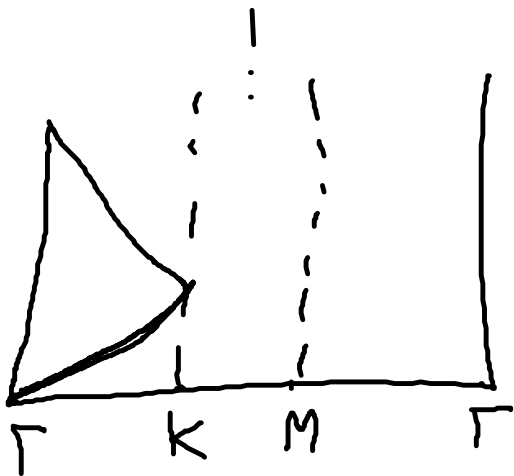
$$n=0: \epsilon_0(\vec{k}) = \frac{\hbar^2}{2m} (k_x^2)$$

$$\epsilon_0(\Gamma) = 0$$

$$\epsilon_0(K) = \frac{\hbar^2}{2m} \left(\frac{2\pi}{a} \frac{1}{\sqrt{3}} \right)^2$$

$$n=2: \epsilon_2(\vec{k}) = \frac{\hbar^2}{2m} \left(k_x^2 + \left(\frac{2\pi}{a} \right)^2 \right)$$

$$\epsilon_2(\Gamma) = \frac{\hbar^2}{2m} \left(\frac{1}{3} + 2 \right) \cdot \left(\frac{2\pi}{a} \right)^2$$



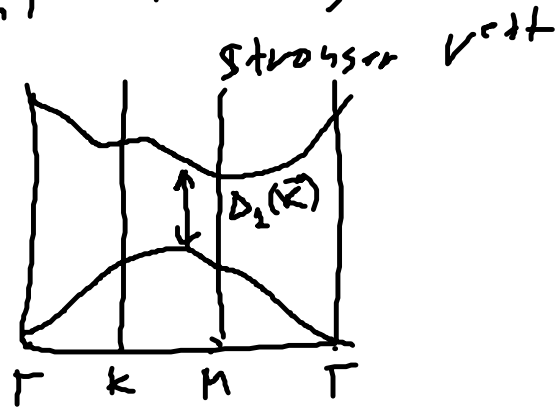
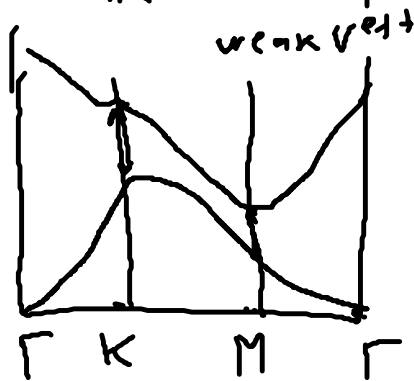
What if $\text{vel}(\vec{G}_n)$ is small $\neq 0$?

$$\frac{1}{\sqrt{N}} e^{i(\vec{k} + \vec{G}_n) \cdot \vec{r}} \rightarrow \begin{cases} \psi_{n\vec{k}}(\vec{r}) = \sum_{\vec{G}_n} C_{\vec{G}_n}(\vec{k}) e^{i(\vec{k} + \vec{G}_n) \cdot \vec{r}} \\ \epsilon_n(\vec{k}) \approx \epsilon_n(\vec{k}) + \Delta_n(\vec{k}) \end{cases}$$

perturbation theory:

$$\Delta_n(\vec{k}) \sim |V^{\text{eff}}(\vec{G}_n)|^2 \text{ for non-degenerate } E_n(\vec{k})$$

$$\Delta_n(\vec{k}) \sim |V^{\text{eff}}(\vec{G}_n)| \text{ for degenerate } E_n(\vec{k})$$



What can we learn from the bandstructure?

- nature of bonding
- chemically active states
- optical properties
- transport properties

Solid with N electrons, $\psi_{n,\vec{k}}(\vec{r})$ can have two electrons: \uparrow, \downarrow

$$E_n(\vec{k}), n \text{ is fixed, } \vec{k} \in \text{BZ}$$

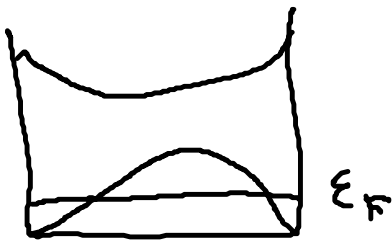
$$2 \int_{\text{BZ}} \frac{V_g}{(2\pi)^3} d^3k \text{ electrons}$$

$$= 2 \frac{V_g}{(2\pi)^3} \cdot \frac{(2\pi)^3}{\Omega} = \frac{2 V_g}{\Omega} = 2N$$

\Rightarrow \uparrow 2 electrons in a band per primitive unit cell
 maximum

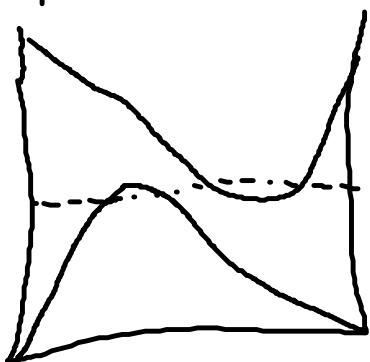
EXAMPLES

- 1) Single valence electron per unit cell
i.e. (Li, Na, Cu, Ag, Au)



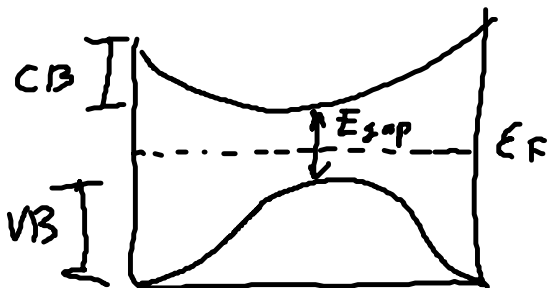
\Rightarrow this material is metallic

- 2) Two electrons per unit cell, $V_{eff} \equiv$ weak



$E_F \Rightarrow$ metal

- 3) Two electrons per unit cell
 $V_{eff} \equiv$ strong



The band gap determines the appearance of the material \Rightarrow metal, semiconductor, insulator

$$E_{gap} = I - A = E^{N-2} + E^{N+2} - 2E^N =$$
$$\approx E_{CB}^{N+\frac{1}{2}} - E_{VB}^{N-\frac{1}{2}} = E_{CB}^N - E_{VB}^N + \Delta^x$$

Visible light $1.65 \text{ eV} < \hbar\omega < 3.1 \text{ eV}$

a) metals $E_{\text{gap}} \ll \hbar\omega$ - visible light

Si : $E_{\text{gap}} = 1.1 \text{ eV}$

GaAs : $E_{\text{gap}} = 1.45 \text{ eV}$

b) E_{gap} is within visible light

GaP (2.35 eV) \rightarrow orange
absorb blue light

c) $E_{\text{gap}} \gg \hbar\omega$ - visible light
Material is transparent

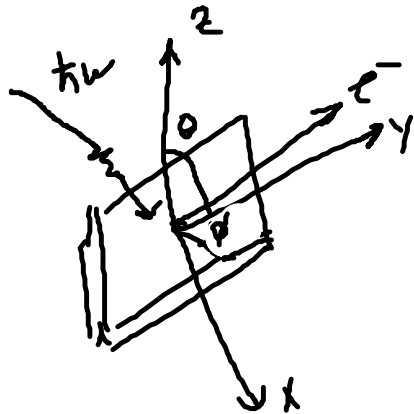
Semiconductors have $E_{\text{gap}} \gtrsim k_B T$.

$T = 300 \text{ K}$ $k_B T = 0.026 \text{ eV}$

Better definition: A semiconductor is an insulator which can be doped to create electrons in the CB or holes in the VB.

The band structure $E_n(\vec{k})$ can be measured by photoemission.

Angular-resolved photoemission:



Measure: $I(\hbar\omega, E_f, \theta, \phi)$

$$E_f \approx E_f - \hbar\omega$$

photoemission measure VB

inverse photoemission measure CB