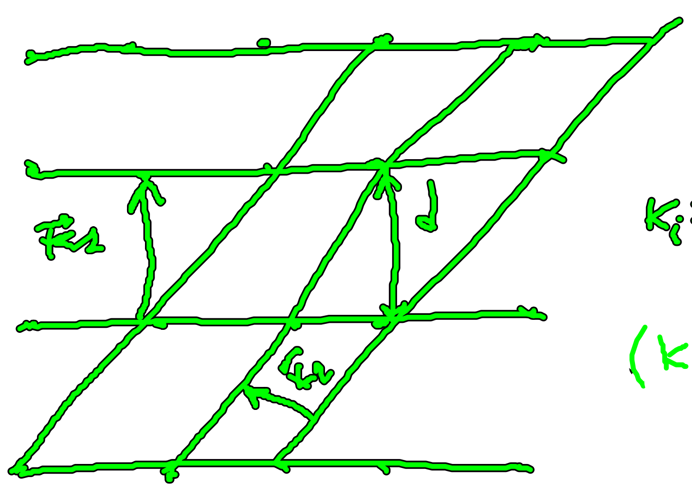
# Reminder (lattice periodicity)

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

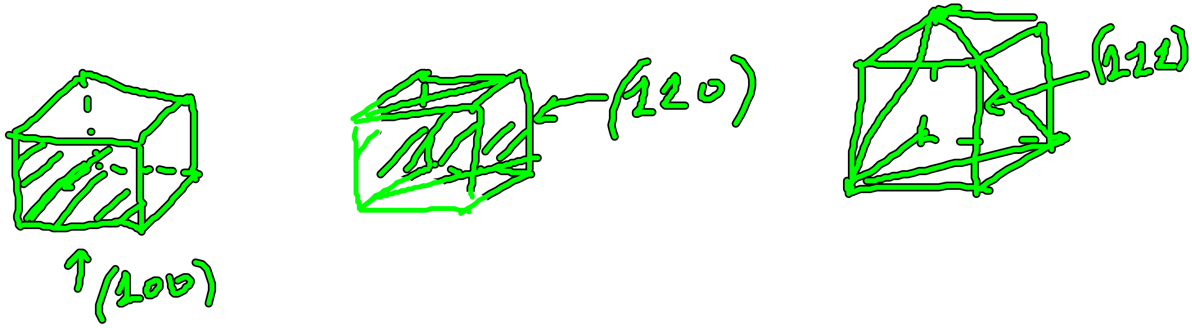
- Bloch theorem $\Leftrightarrow$ $\vec{k}$ appears
- Reciprocal space and Brillouin zone

Side view of a crystal

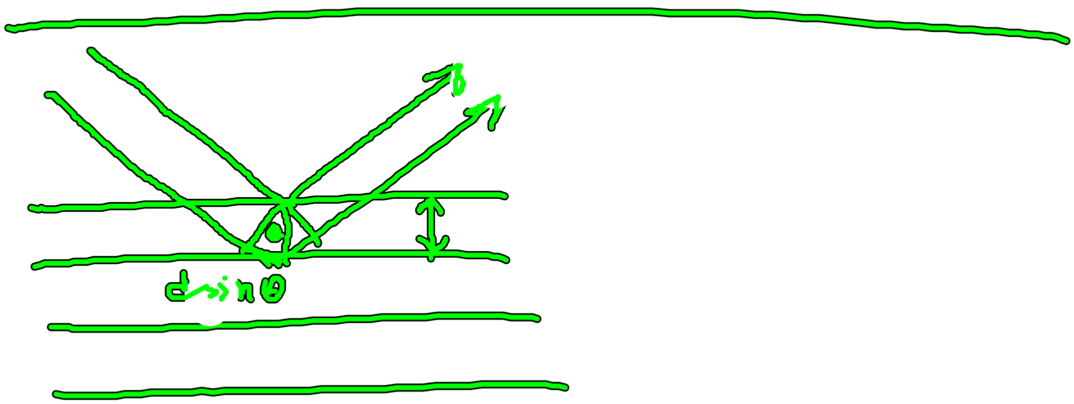



$$k_i = \frac{2\pi}{d_i}$$

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




Connection to reflection (photons or electrons)




Condition of reflection => Bragg condition

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

$\lambda \equiv$ wavelength

$\vdots$

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

## Chapter 5 Band structure of the electrons

$$\psi_{\vec{K}}(\vec{r}) = \sum_m c_{\vec{G}_m}(\vec{K})\, e^{i(\vec{K}-\vec{G}_m)\vec{r}}$$

$$h_{n,m} = \frac{\hbar^2}{2m}(\vec{K}+\vec{G}_m)^2\,\delta_{n,m} + V^{eff}(\vec{G}_m - \vec{G}_n)$$

$\Rightarrow \quad \mathcal{E}_n(\vec{k}) \qquad \frac{2\pi}{a}(0,1)$

What happens in 2D? $\quad \vec{G}_2 = \frac{2\pi}{a}\left(\frac{\sqrt{3}}{2}, \frac{1}{2}\right)$

Example:


if all components of $V^{eff}(G_n)$ are small

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

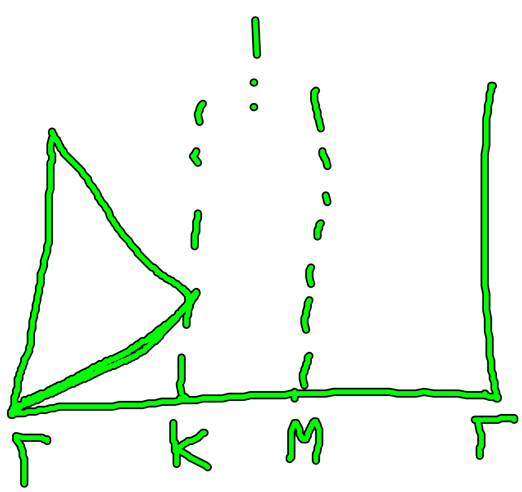
$n=0$: $\quad \mathcal{E}_0(\vec{k}) = \frac{\hbar^2}{2m}(k_x^2)$

$$\mathcal{E}_0(\Gamma) = 0$$

$$\mathcal{E}_0(K) = \frac{\hbar^2}{2m}\left(\frac{2\pi}{a}\frac{1}{\sqrt{3}}\right)^2$$

$n=1$: $\quad \mathcal{E}_1(\vec{k}) = \frac{\hbar^2}{2m}\left(k_x^2 + \left(\frac{2\pi}{a}\right)^2\right)$

$$\mathcal{E}_1(\Gamma) = \frac{\hbar^2}{2m}\left(\frac{1}{3}+1\right)\cdot\left(\frac{2\pi}{a}\right)^2$$



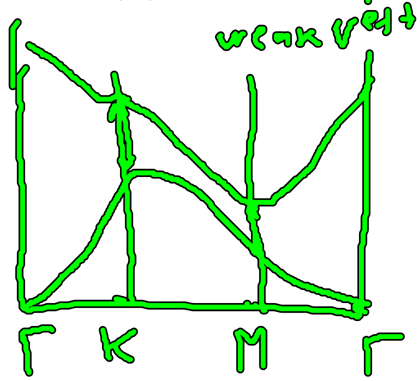

what if $V^{eff}(G_n)$ is small $\neq 0$?

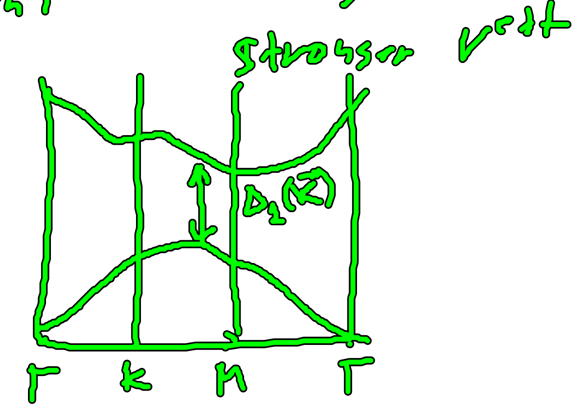
$$\frac{1}{\sqrt{V_g}} e^{i(\vec{k}+\vec{G}_n)\vec{r}} \longrightarrow \begin{cases} \psi_{n\vec{k}}(\vec{r}) = \sum_{\ell} C_{\vec{G}_n}(\vec{k})\, e^{i(\vec{k}+\vec{G}_\ell)\vec{r}} \\ \mathcal{E}_n(\vec{k}) \simeq \mathcal{E}_n(\vec{k}) + \Delta_n(\vec{k}) \end{cases}$$

perturbation theory:

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

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




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: ↑, ↓

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

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

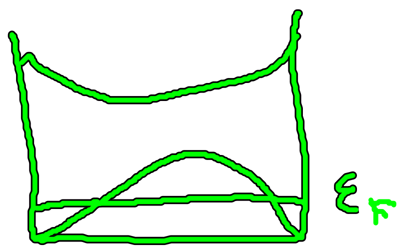
$$= 2\frac{V_g}{(2\pi)^3}\cdot\frac{(2\pi)^3}{\Omega} = \frac{2V_g}{\Omega} = 2\hat{N}$$

$\Rightarrow$ 2 electrons in a band per primitive unit cell

maximum

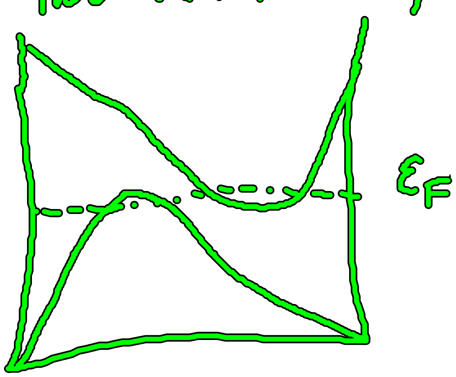
# EXAMPLES

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



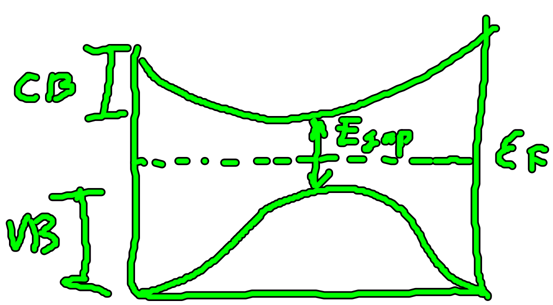

$\Rightarrow$ this material is metallic

2) Two electrons per unit cell, $V^{eff} \equiv$ weak




$\Rightarrow$ metal

3) Two electrons per unit cell
$V^{eff} \equiv$ strong

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

$$E_{gap} = I - A = E^{N-1} + E^{N+1} - 2E^{N} =$$

$$\approx \varepsilon_{CB}^{N+\frac{1}{2}} - \varepsilon_{VB}^{N-\frac{1}{2}} = \varepsilon_{CB}^{N} - \varepsilon_{VB}^{N} + \Delta^{xc}$$

Visible light $1.65\,eV < \hbar\omega < 3.1\,eV$

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

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

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

b) $E_{gap}$ is within visible light

GaP ( 2.35 eV ) $\rightarrow$ orange

absorb blue light

c) $E_{gap} \gg \hbar\omega$ - visible light

Material is transparent

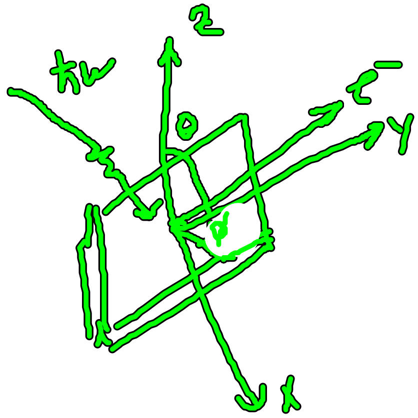
Semiconductors have $E_{gap} \gtrsim k_B T$.

$T = 300K$ $\quad k_B T = 0.026\ eV$

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: $I(\hbar\omega, \varepsilon_f, \theta, \phi)$

$\varepsilon_f \simeq \varepsilon_g - \hbar\omega$

photoemission measures VB

inverse photoemission measures CB