VE 320 Summer 2019

Introduction to Semiconductor Devices

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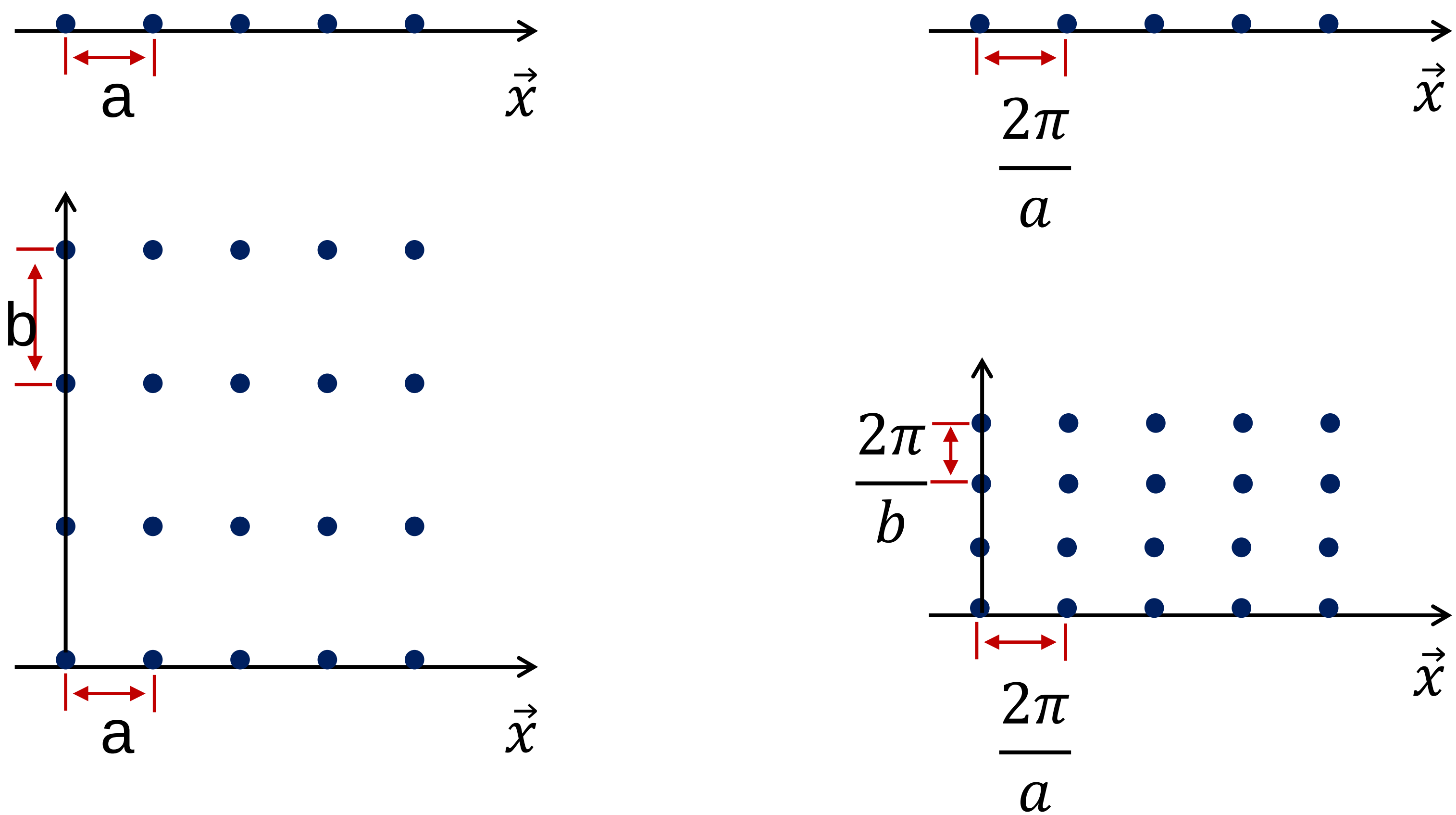
Lecture 3

Introduction to quantum theory of solids (Chapter 3)

Reciprocal Lattice

Real space → Reciprocal space (k space)



Reciprocal Lattice

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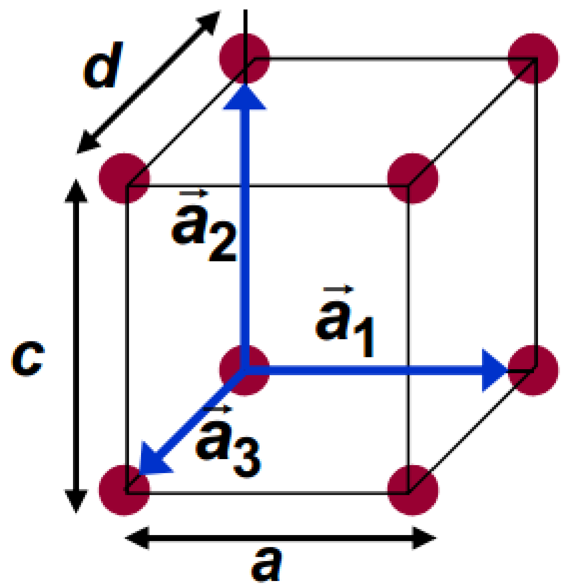
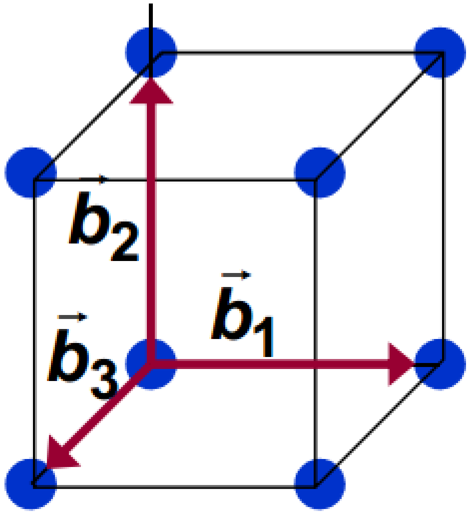
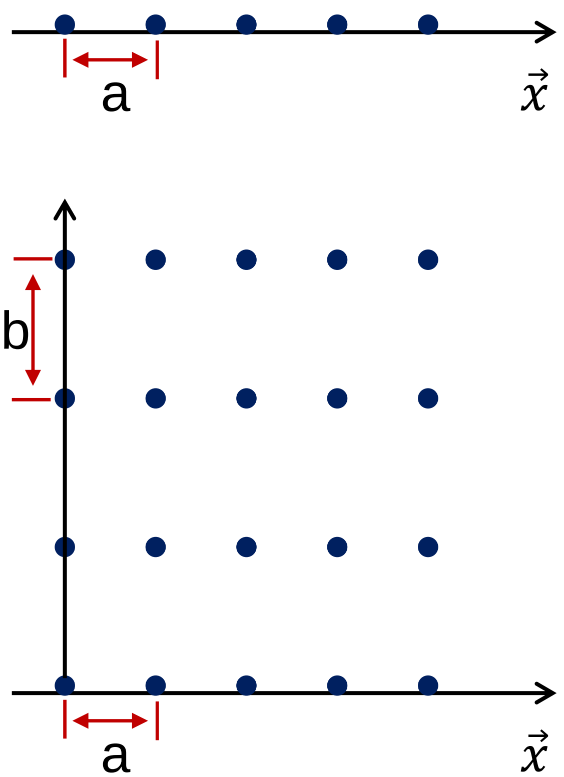


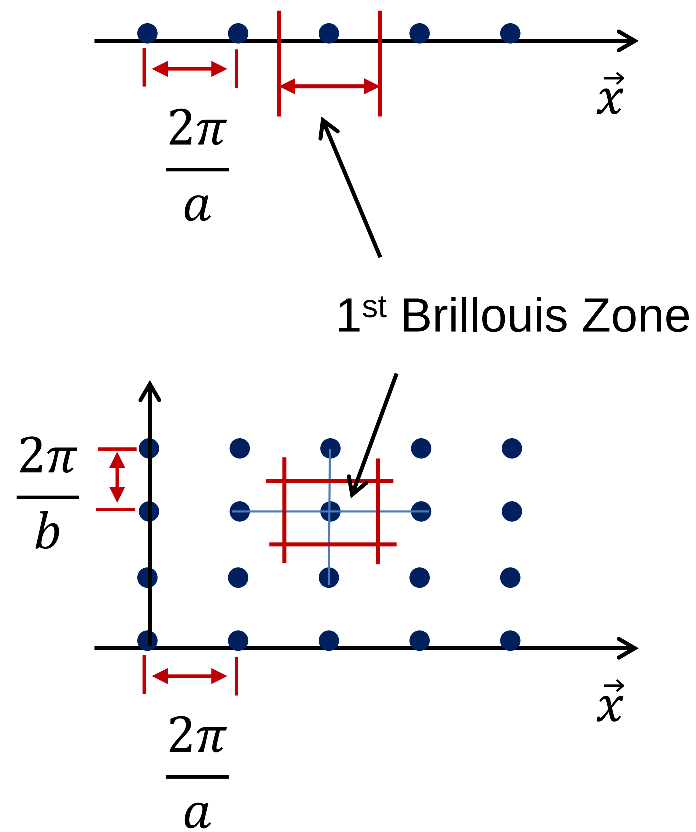


$$\overrightarrow{b_1} = \frac{2\pi}{a_1}\hat{x} \qquad \overrightarrow{b_2} = \frac{2\pi}{a_2}\hat{y} \qquad \overrightarrow{b_3} = \frac{2\pi}{a_3}\hat{z}$$

Brillouin zone

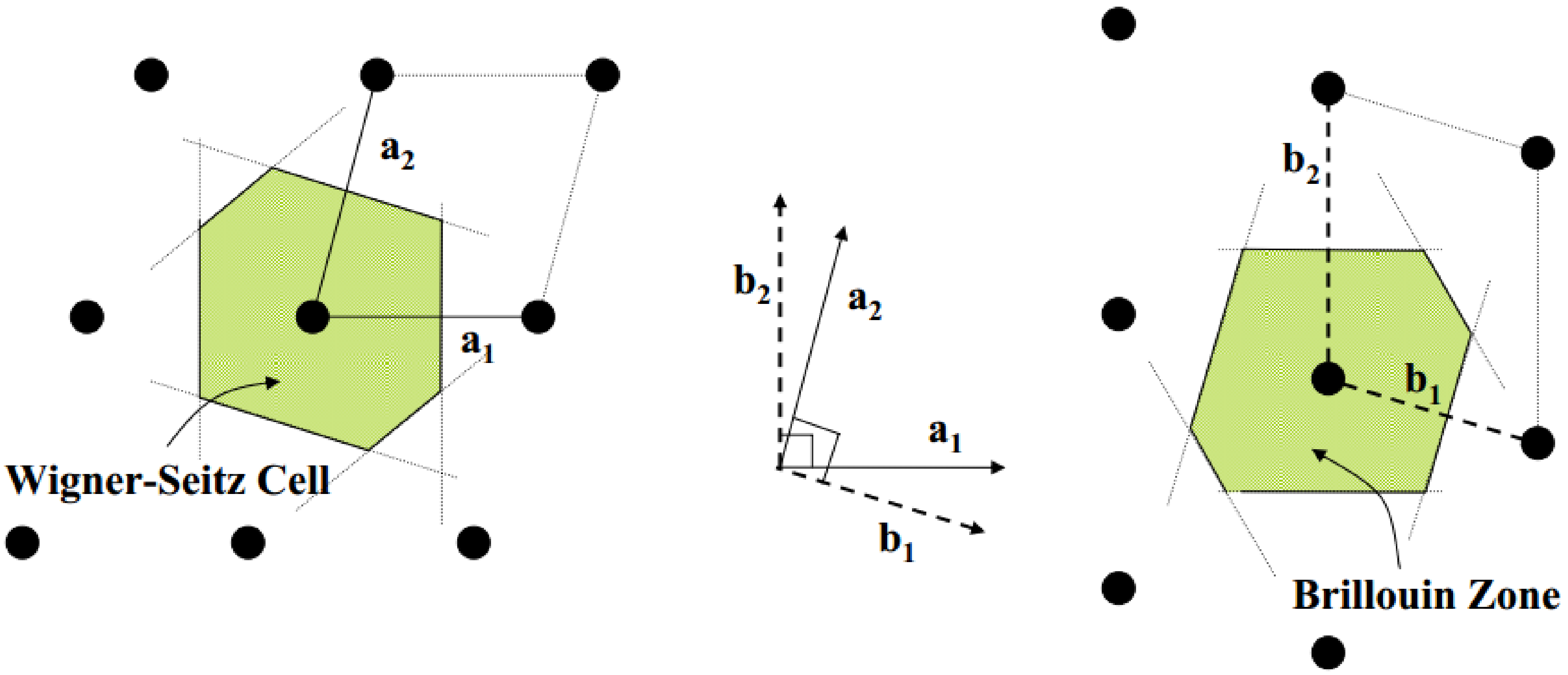
Real space → Reciprocal space (k space)





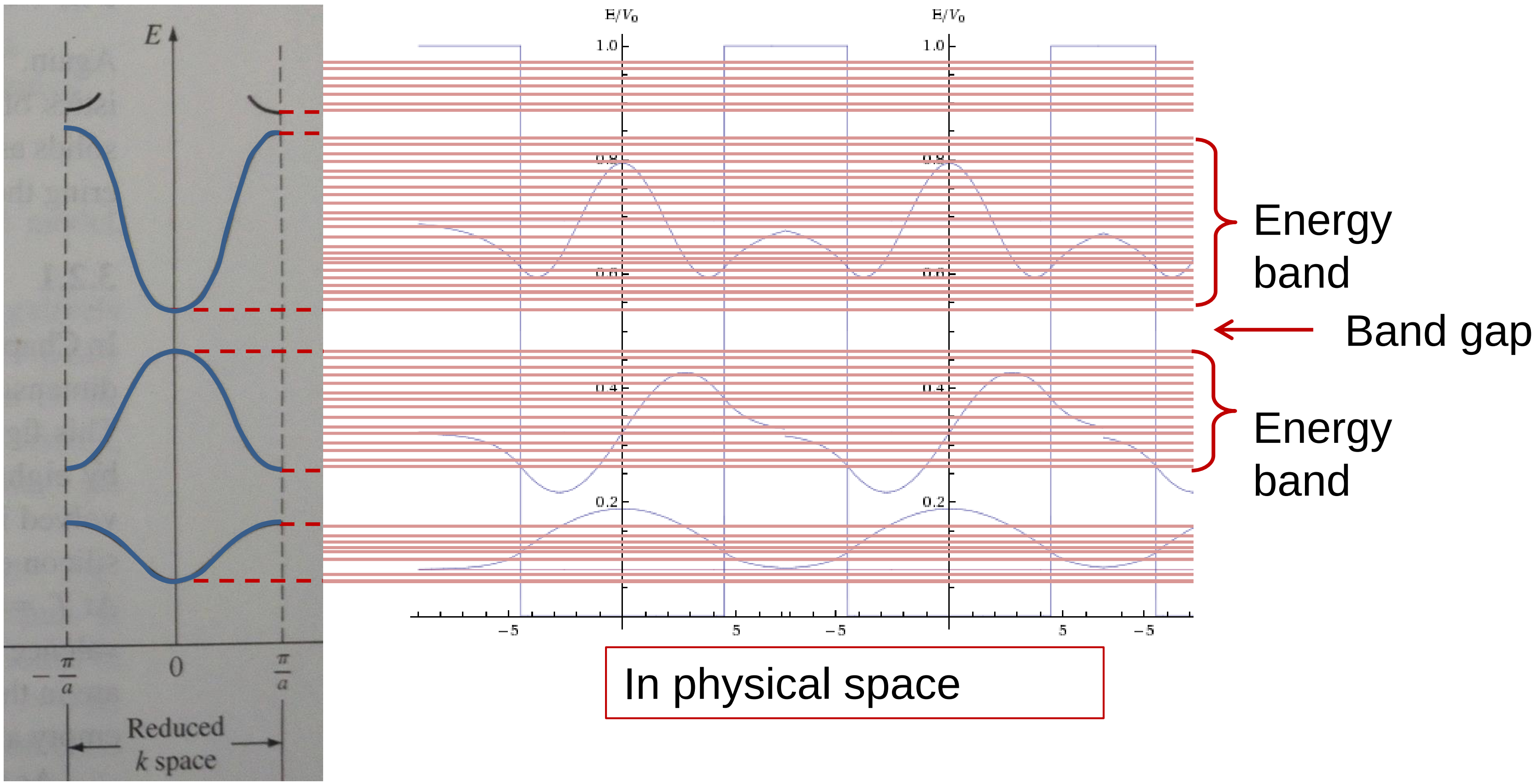
Brillouis zone

Real & Reciprocal lattices in 2 D



Previously…

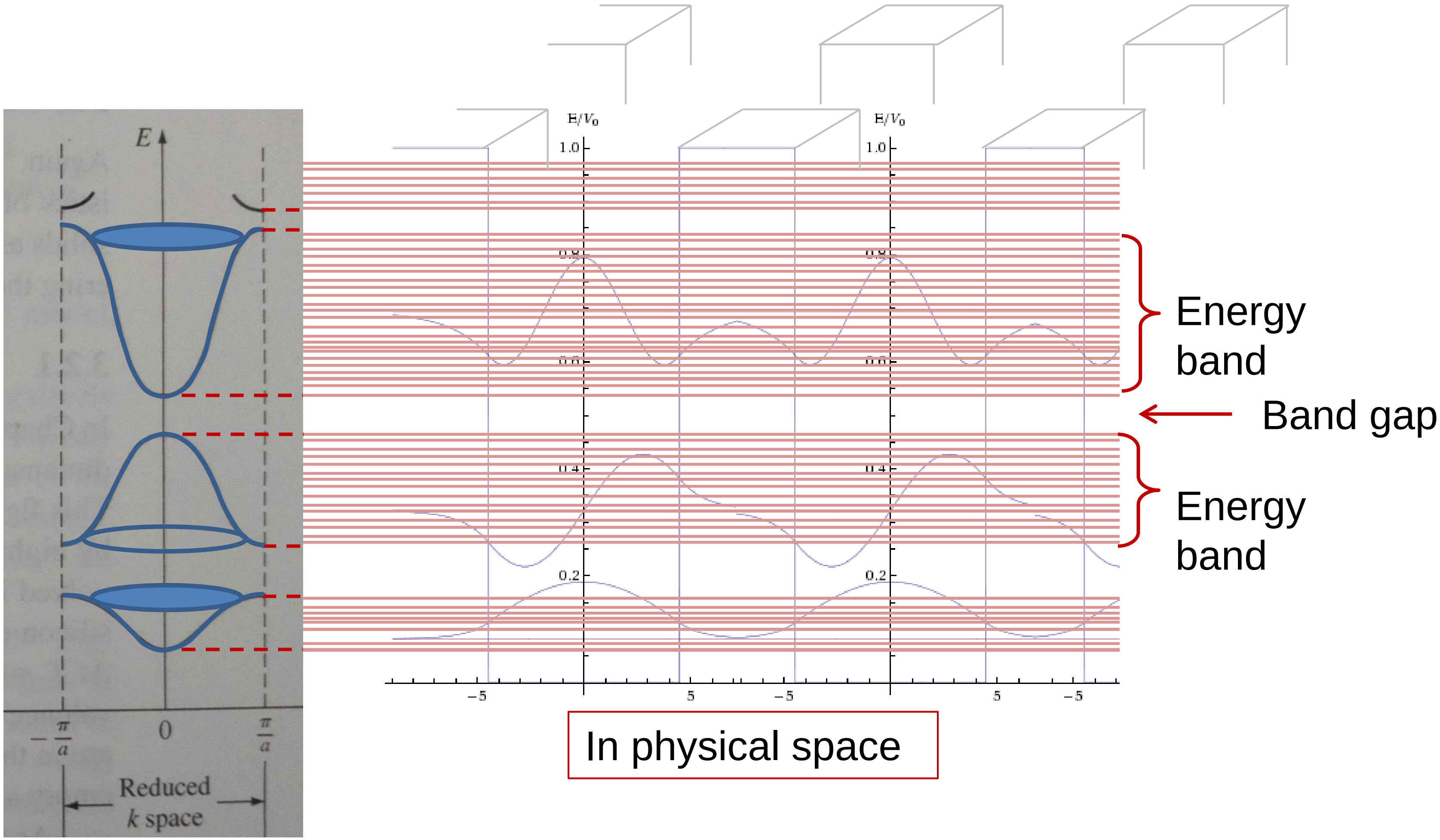
Band structure in physical and k space for 1D periodic quantum wells



In k space

In physical space

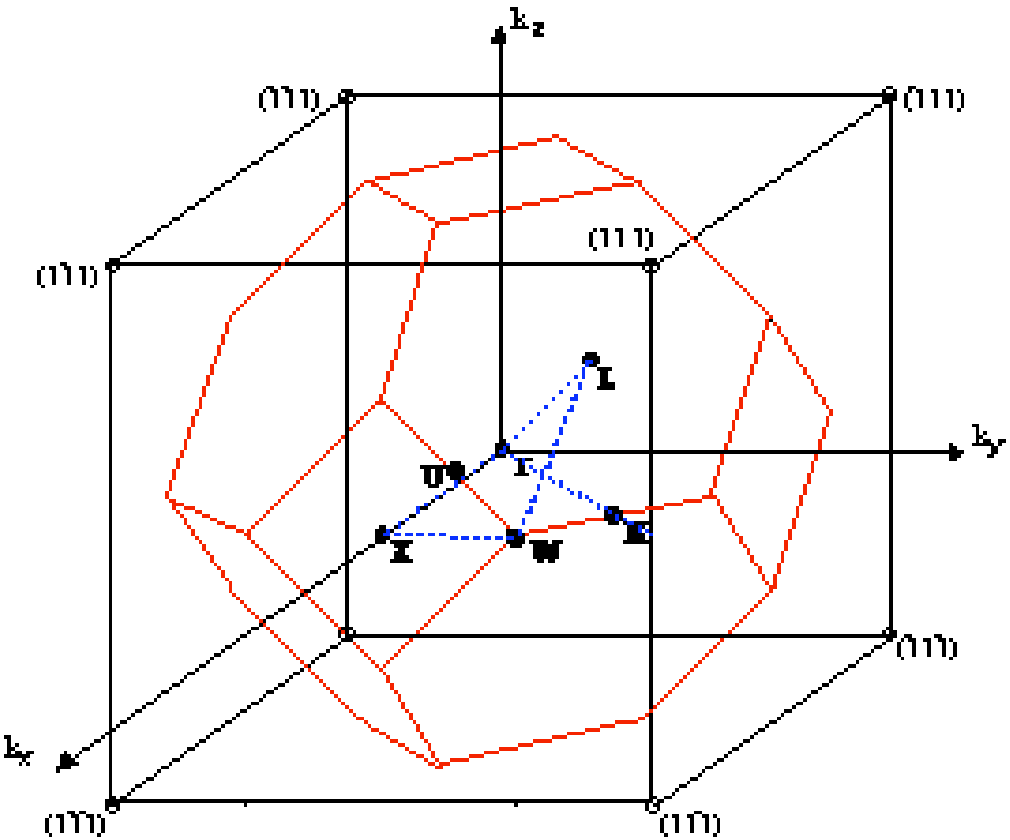
2D periodic potential well



In physical space

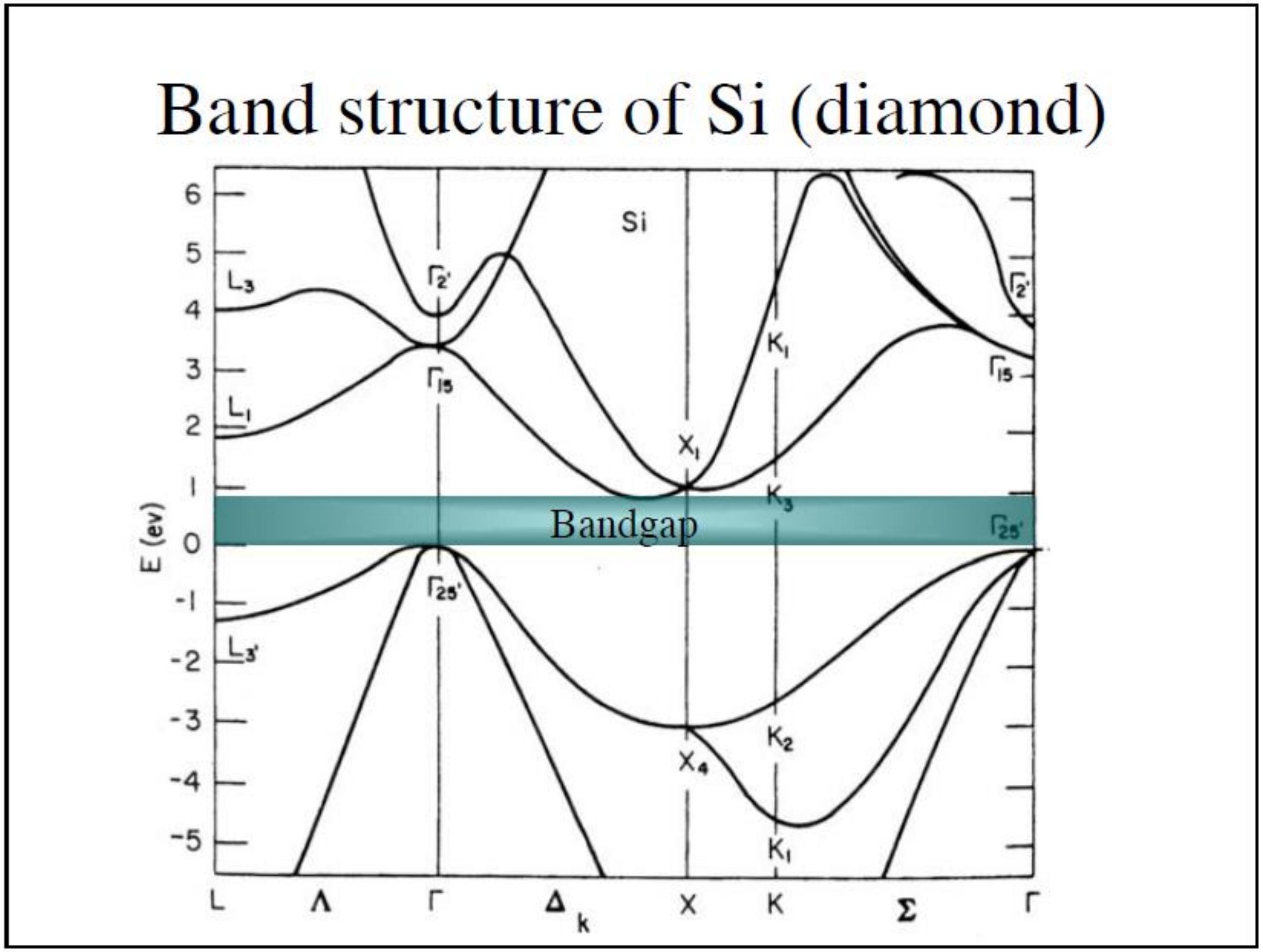
In k space

Band structure in 3D k-space



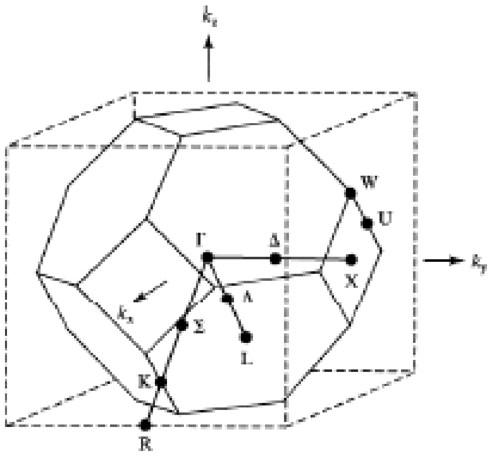
Γ - center of the BZ
X - [100] intercept; Γ – X path Δ
K - [110] intercept; Γ – K path ∑
L - [111] intercept; Γ – L path Λ

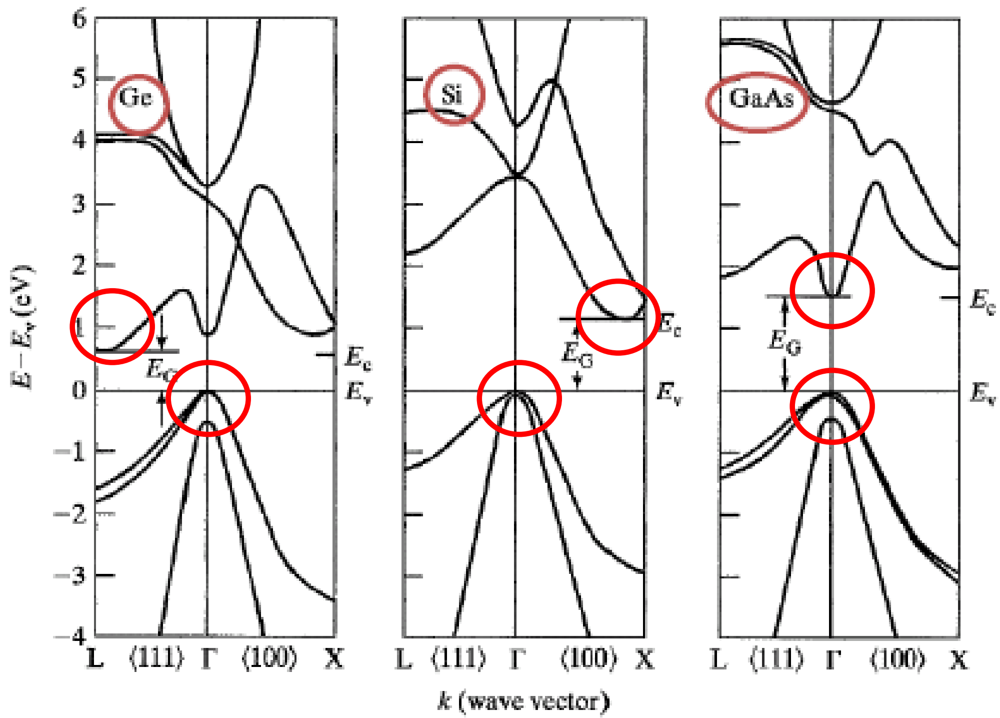
Band structure in 3D k-space



Why is it so complicated?

Band structure in 3D k-space



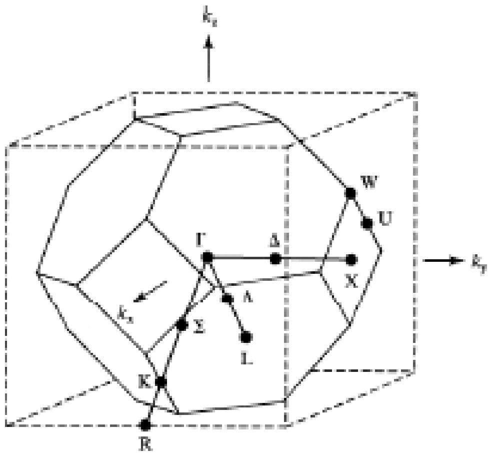


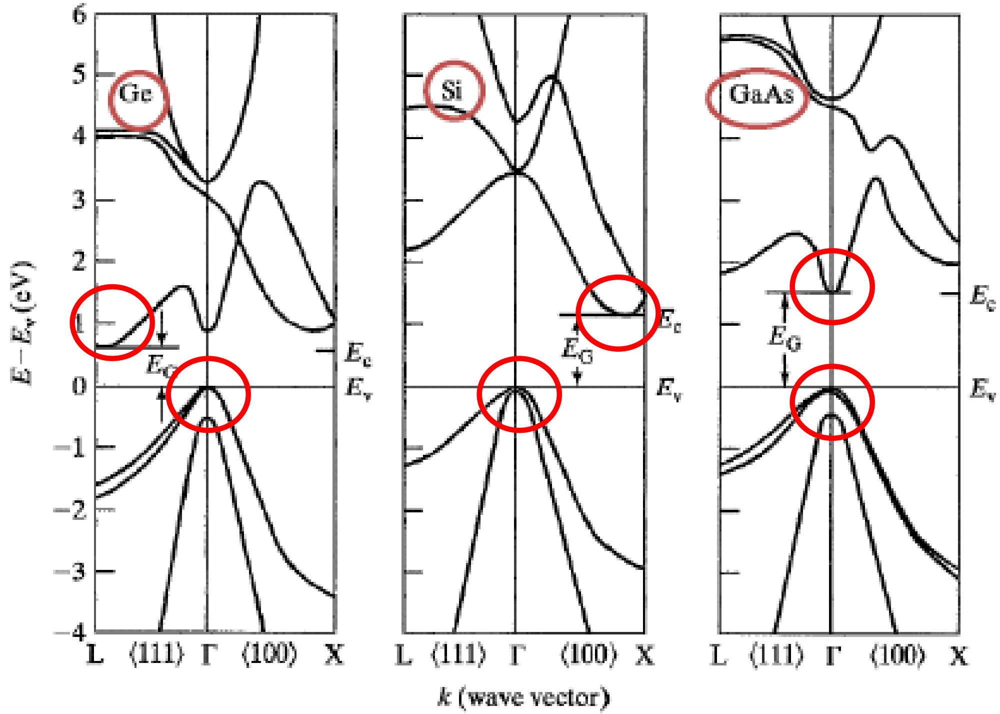
- Direct bandgap

  (electron excited, k constant, E↑ → f ↑, v = f λ↑)

- Indirect bandgap

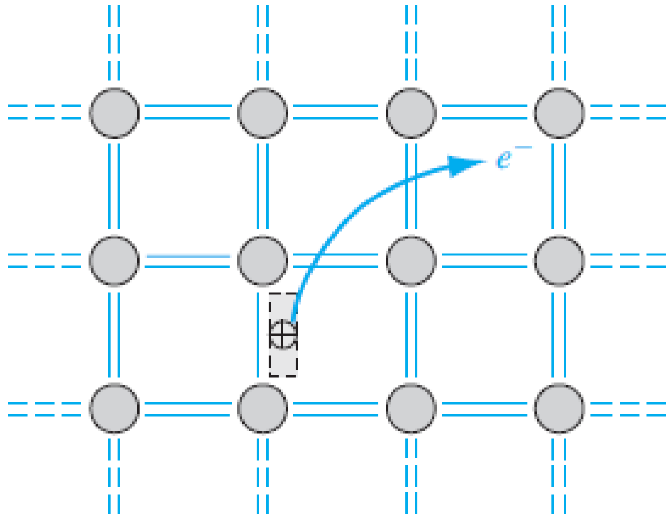
Effective mass of electrons

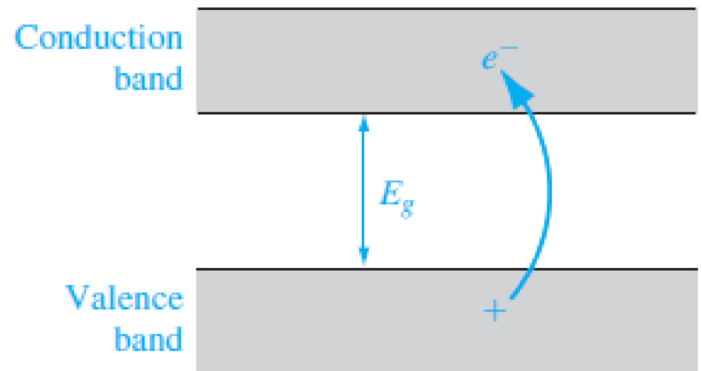




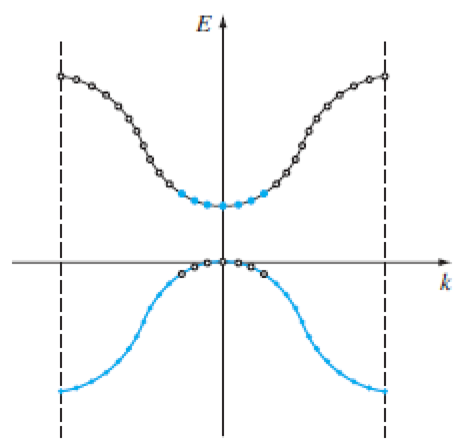
- So far the energy band structure is theoretically calculated.
- How to experimentally find it?

Thermally excited bond breaking in Si





T>0 K



Drift current

$$J = qNv_d \qquad \text{A/cm}^2$$

Positively charged ions with a volume density *N* (cm^{-3}) and an **average** drift velocity v_d (cm/s).

$$J = q\sum_{i=1}^{N} v_i$$

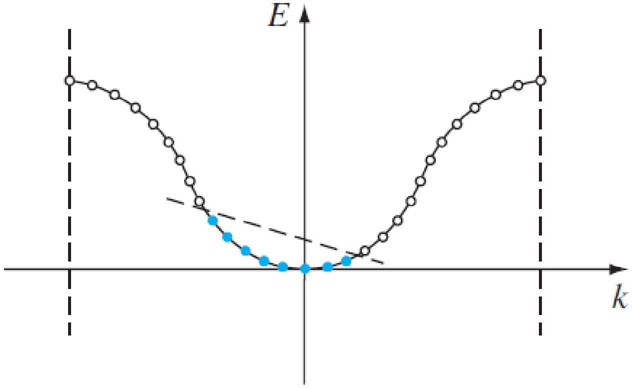
Individual drift velocity v_i (cm/s).

Zero electric field: next drift current = 0
When electric field is applied:

$$dE = F\,dx = F\,v\,dt$$

F: force, *E*: energy

$$J = -e\sum_{i=1}^{n} v_i$$



Effective mass

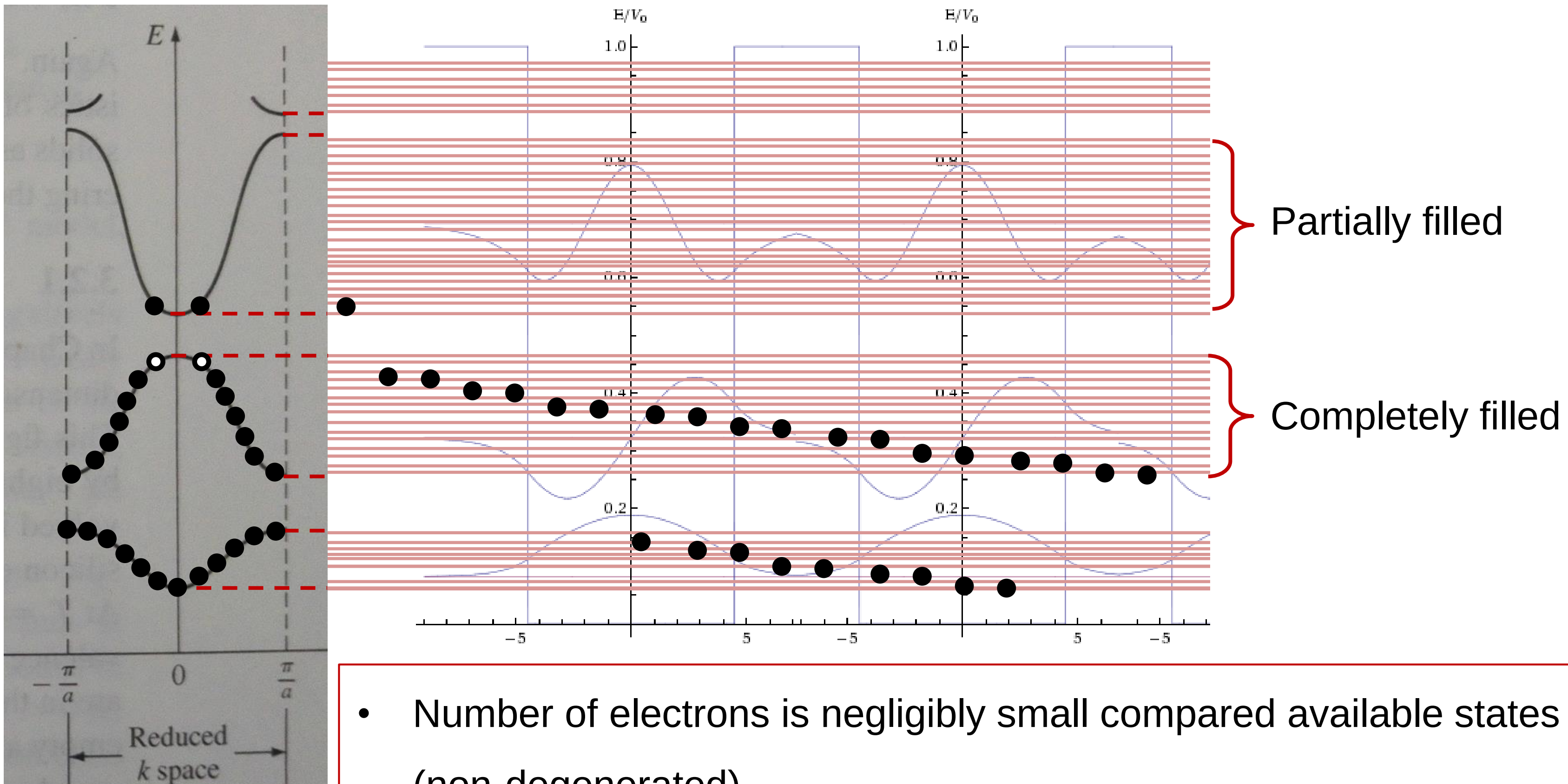
Internal forces in the crystal due to positively charged ions or protons and negatively charged electrons, which will influence the motion of electrons in the lattice.

$$F_{\text{ext}} = m^* a$$

m*: effective mass, takes into account the effect of the internal forces
Relates the quantum mechanical results to the classical force equations.
In most instances, the electron in the bottom of the conduction band can be thought of as a classical particle through the use of the effective mass.

Effective mass of electrons

Semiconductors

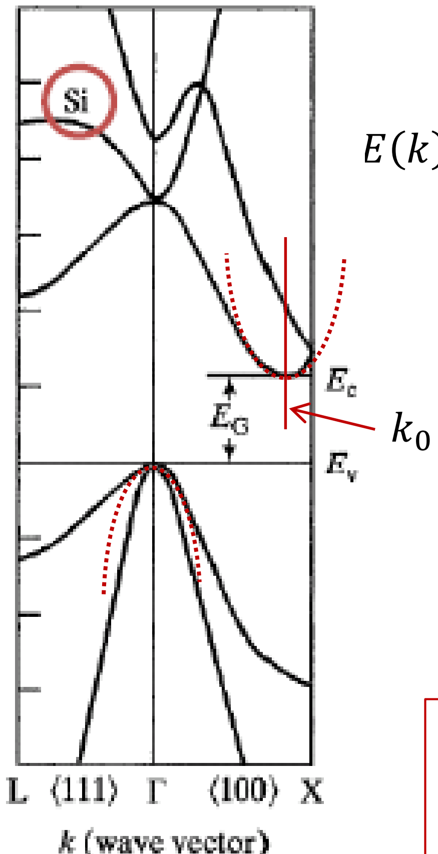


In k space

- Number of electrons is negligibly small compared available states (non-degenerated)
- Electrons mostly located at the bottom of conduction band

Effective mass of electrons

Semiconductors



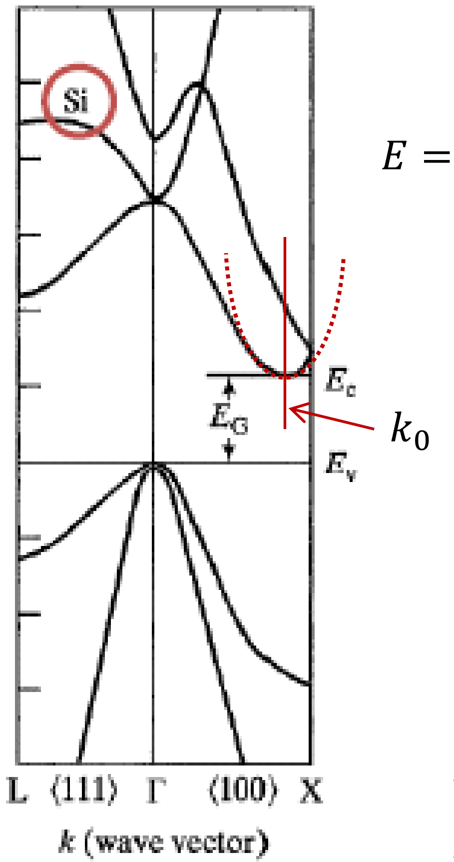
$$E(k) = E(k = k_0) + \frac{dE}{dk}|_{k=k_0}(k - k_0) + \frac{d^2E}{2dk^2}|_{k=k_0}(k - k_0)^2 + O((\Delta k)^3)$$

Taylor series

- Number of electrons is negligibly small compared available states (non-degenerated)
- Electrons mostly located at the bottom of conduction band

Effective mass of electrons

Semiconductors



$$E = E(k) = E(k = k_0) + \frac{dE}{dk}|_{k=k_0}(k - k_0) + \frac{d^2E}{2dk^2}|_{k=k_0}(k - k_0)^2 + O((\Delta k)^3)$$

For electrons in free space:

$$E = \frac{\hbar^2 k^2}{2m} \Rightarrow \frac{d^2E}{dk^2} = \frac{\hbar^2}{m} \qquad \frac{d^2E}{dk^2}|_{k=0} = \frac{\hbar^2}{m} \qquad \frac{1}{\hbar^2}\frac{d^2E}{dk^2} = \frac{1}{m}$$

For electrons with energy near the bottom of the energy band:
E-*k* relationship can be approximated by a parabola

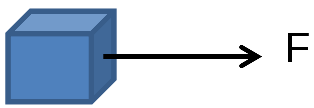
$$\frac{1}{\hbar^2}\frac{d^2E}{dk^2} = \frac{2C_1}{\hbar^2} = \frac{1}{m^*}$$

- m* has a unit of mass, positive for electron
- We call it the effective mass for electrons in the crystal

Effective mass of electrons

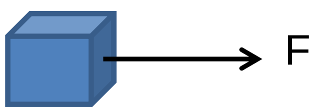
- How to understand effective mass

Example: use Newton's law to find mass of an object



$$m = \frac{F}{a} \qquad a = \frac{d^2x}{dt^2}$$

In the air



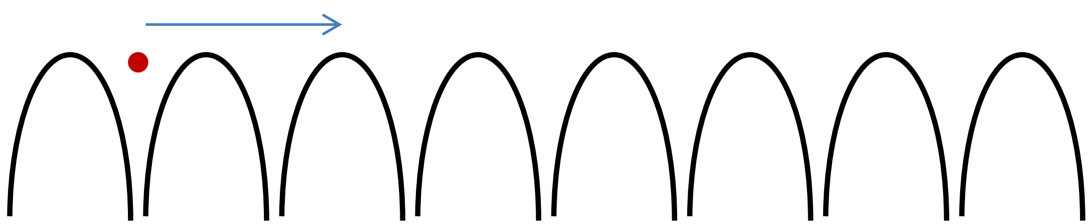
$$m^* = \frac{F}{a} \qquad a = \frac{d^2x}{dt^2}$$

In the water

Effective mass of electrons

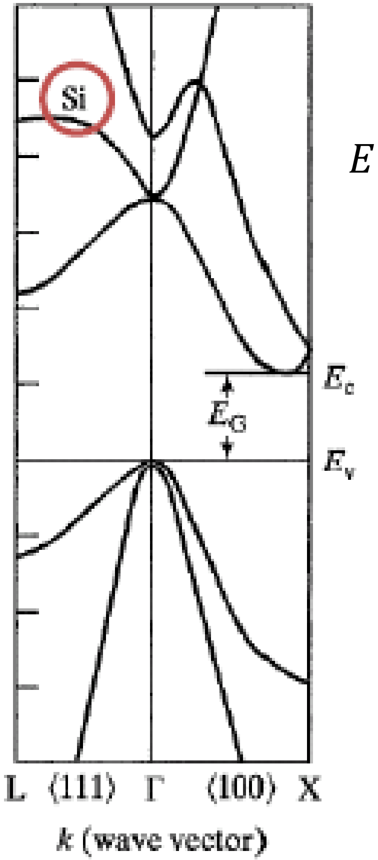
- How to understand effective mass

Modulated by Electric potential of ions



Effective mass of electrons

Semiconductors



For Electrons in the conduction band:

$$E = E(k) = E(k = k_0) + \frac{dE}{dk}|_{k=k_0}(k - k_0) + \frac{d^2E}{2dk^2}|_{k=k_0}(k - k_0)^2 + O((\Delta k)^3)$$

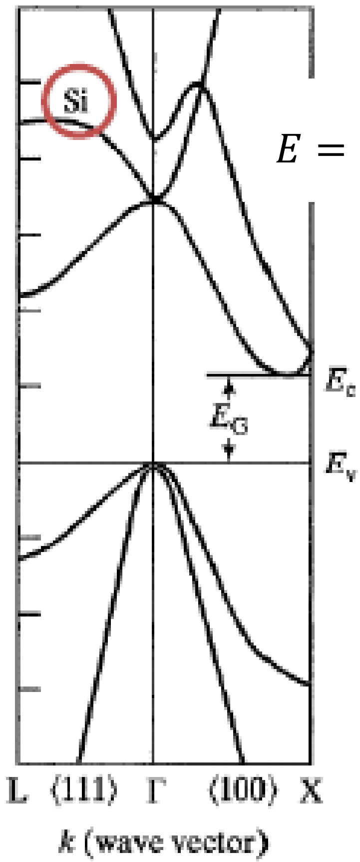
$$\boxed{E = E(k) = E_c + \frac{\hbar^2}{2m_n^*}k^2}$$

For Electrons in the valence band:

$$\boxed{E = E(k) = E_c - \frac{\hbar^2}{2m_p^*}k^2}$$

Effective mass of electrons

Semiconductors



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For Electrons in the valence band:

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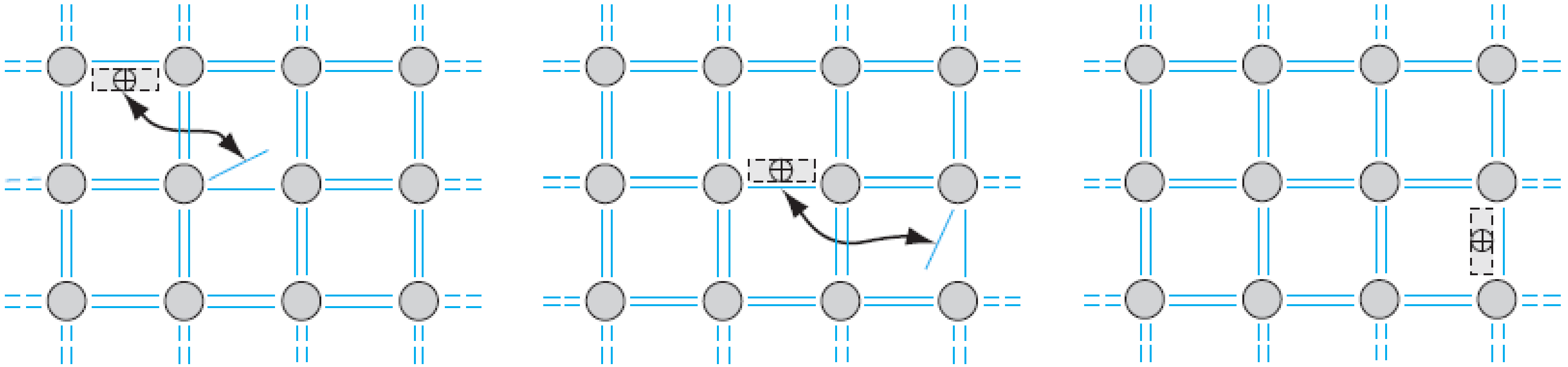
New charge carrier: holes

- Equivalent to a positive charge carrier
- Different effective mass
- Electrons and holes can come from dopants separately

Effective mass of holes



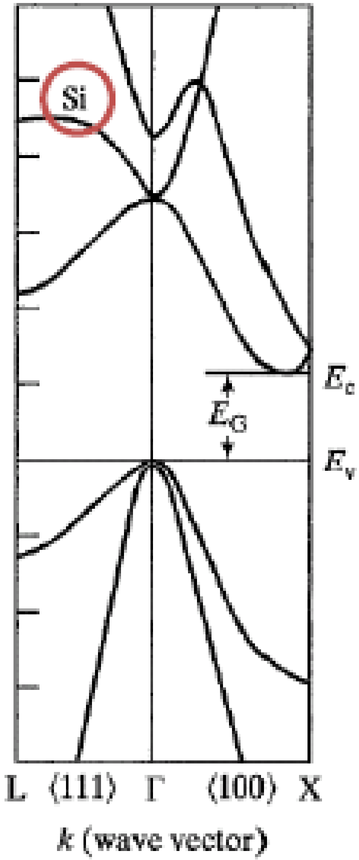
Movement of valence electrons in the crystal, alternately filling one empty state and creating a new empty state—a motion equivalent to a positive charge moving in the valence band. The crystal now has a second equally important charge carrier that can give rise to a current. This charge carrier is called a *hole*

$$\frac{1}{\hbar^2}\frac{d^2E}{dk^2} = \frac{-2C_2}{\hbar^2} = \frac{1}{m^*}$$

- m*: negative, an electron moving near the top of an allowed energy band moves in the same direction as the applied electric field.
- Hole: positive effective mass denoted by m_p^* and a positive electronic charge.

Effective mass of electrons

Semiconductors



- If we can experimentally measure the effective mass, we will have found the analytical expression of energy band structure for non-degenerated semiconductors.
- How?

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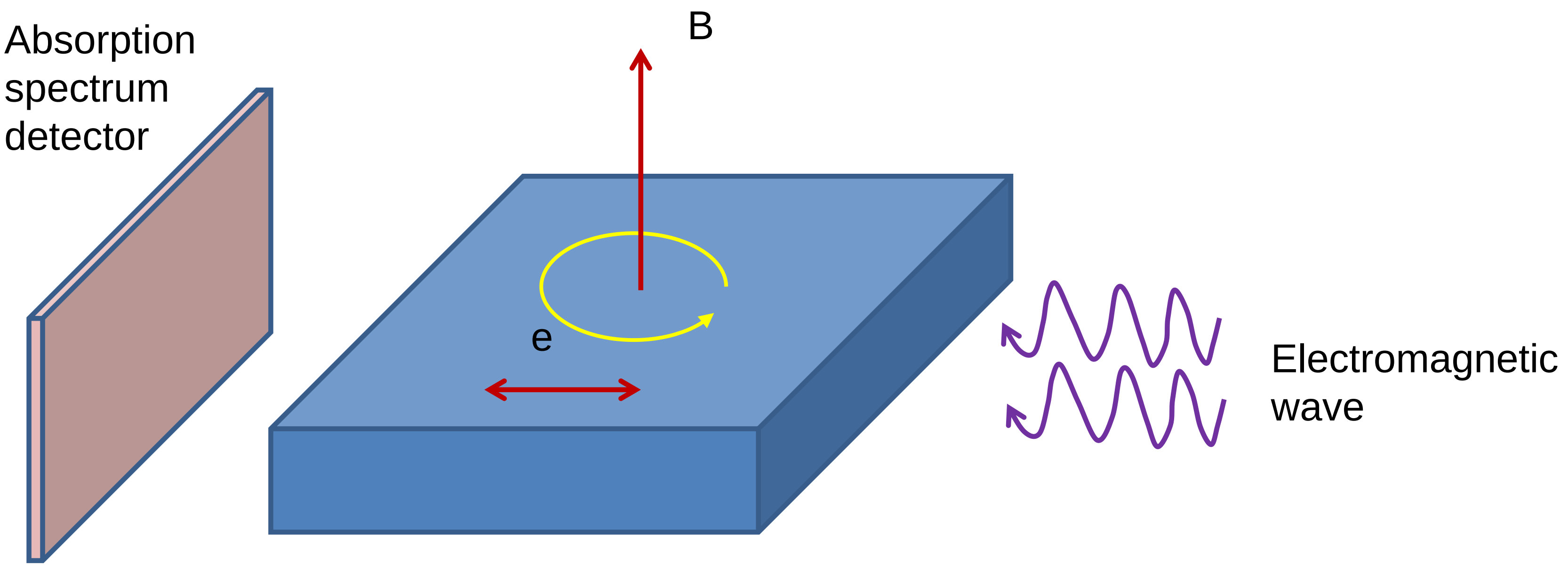
Effective mass of electrons

- Electron Spin Resonance



Effective mass of electrons

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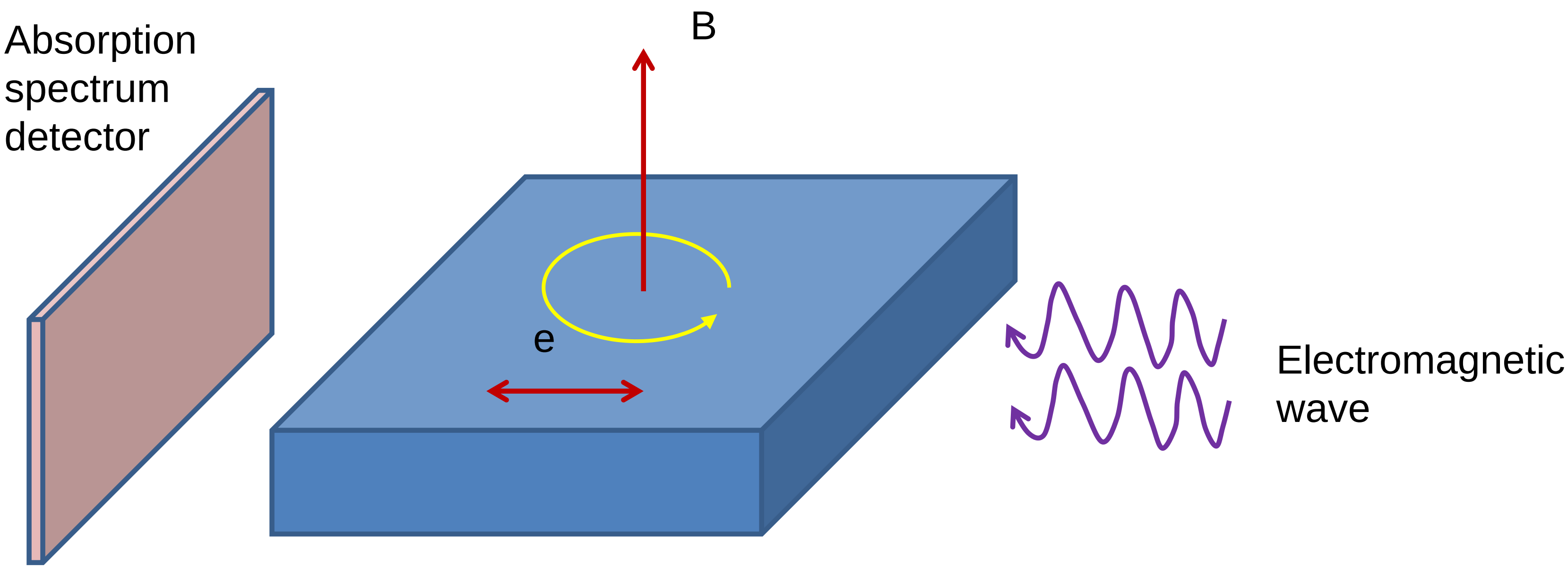
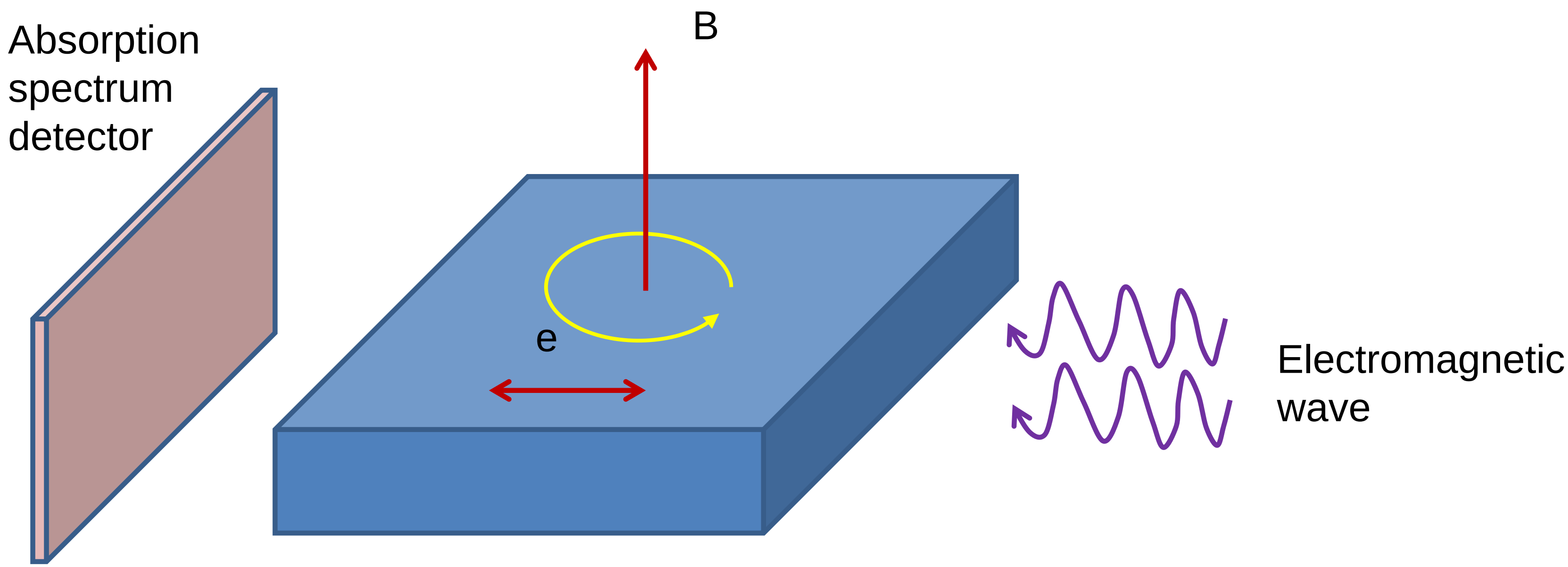


Suppose a intrinsic silicon wafer is placed in a magnetic field B = 1T. We find a dip at λ=5mm in the absorption spectrum, what is the effective mass of electrons? The mass of electrons in free space m_0 = 9.1e-31kg.

Effective mass of electrons

- Electron Spin Resonance

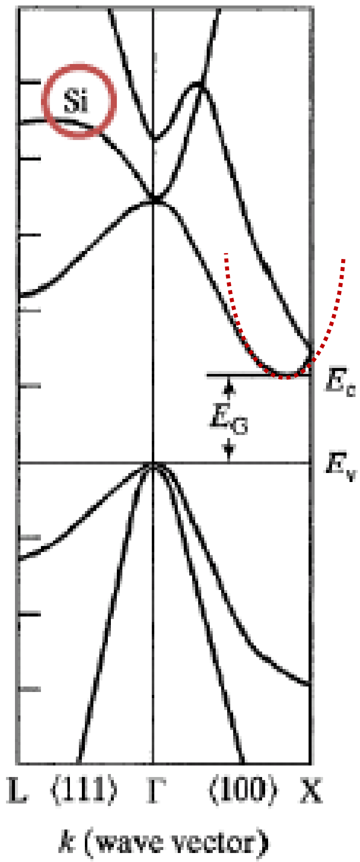


Centrifugal force $F = m^* \omega^2 r$ ➡ $m^*=eB/\omega$ $\omega = 2\pi f$

Magnetic force $F_{mag} = e \times v \times B$

$v = \omega r$ ➡ $m^* = \frac{eB\lambda}{2\pi c} = \frac{1.6 \times 10^{-19} \times 0.005}{2\pi \times 3 \times 10^8} = 0.47 m_0$

Effective mass of electrons



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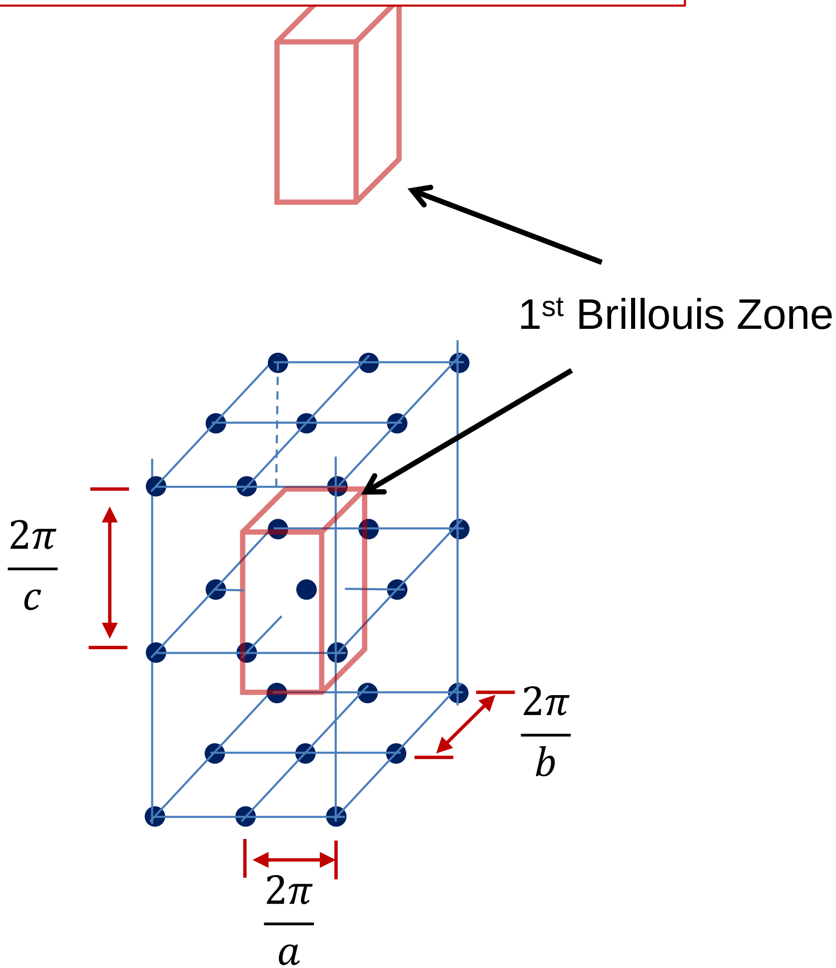
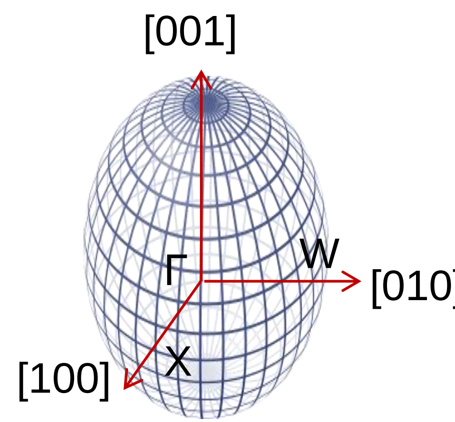
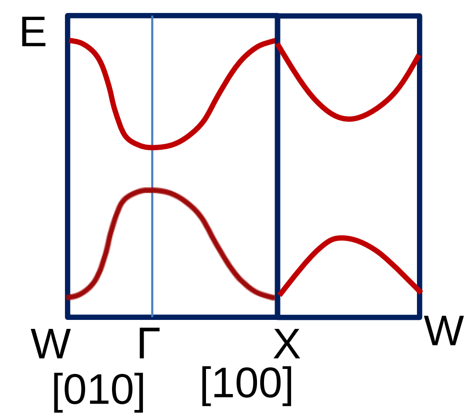
Band structure in 3D k-space

$$E = E(k) = E_c + \frac{\hbar^2}{2}\left(\frac{k_x^2}{m_{nx}^*} + \frac{k_y^2}{m_{ny}^*} + \frac{k_z^2}{m_{nz}^*}\right)$$



Equal energy "surface"





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Band structure in 3D k-space

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$$m_n^* = \sqrt{m_{nx}^{*2} + m_{ny}^{*2} + m_{nz}^{*2}}$$