Course 2

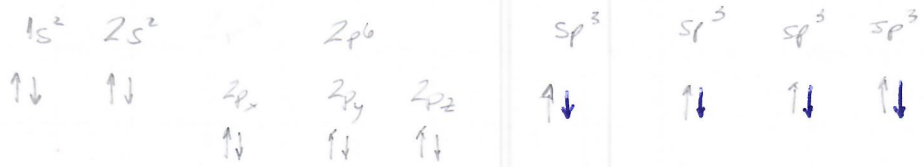
Let us consider a Silicon atom:

#4 14 electrons : $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^2$ — for a single atom

But in a crystal

$3s^2\ 3p^2$ hybridize to form 4 sp^3 hybrid orbitals

⇓ represent the 4 covalent bonds



form a tetrahedral structure

#6 How many Silicon atoms per cm^3:

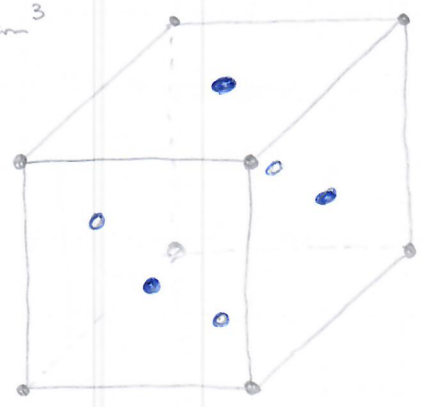
corners : $8 \times 1/8 = 1$

faces : $6 \times 1/2 = 3$ ⇒ 8 atoms

inside : 4

cell volume : $(5.431 \times 10^{-10}\ m)^3 = (5.431 \times 10^{-8}\ cm)^3 = 1.60 \times 10^{-22}\ cm^3$

$\therefore \quad \frac{8}{1.60 \times 10^{-22}} = 5 \times 10^{22}$ atoms / cm^3

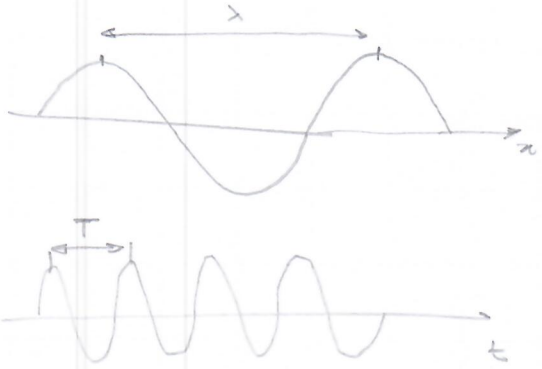


Dual nature of electrons :

if electrons are a wave, we can define a wavevector :

$$\Psi(x,t) = A \cdot \cos(Kx - \omega t + \varphi)$$

$$K = \frac{2\pi}{\lambda} \quad , \quad \omega = \frac{2\pi}{T}$$



The wave nature of electrons is only relevant when $\lambda_B \sim$ dimensions of the system.

→ De Broglie wavelength : $\lambda_B = \frac{h}{p}$

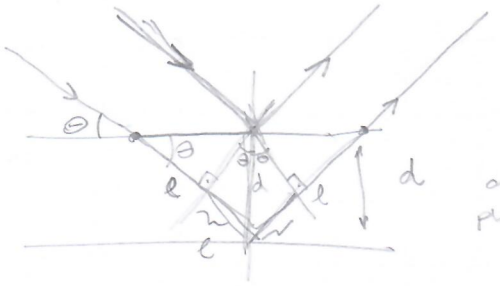
for a free electron at room temperature (RT) :

$$p = \sqrt{2 m_e \cdot E_c} = \sqrt{2 \cdot 5.69 \times 10^{-16} \frac{eV \cdot s^2}{cm^2} \cdot 0.026\ eV}$$

m_e ; $K \cdot T$ ↓ thermal energy

$$\lambda_B = \frac{4.14 \times 10^{-15}\ eV \cdot s}{\sqrt{2 \cdot 5.69 \times 10^{-16} \frac{W s^2}{cm^2} \cdot 0.026\ eV}} = 7.6 \times 10^{-7}\ cm = 7.6\ nm$$

Bragg Law :



Extra distance :

$$2\ell = 2d\sin\theta$$

if $2\ell = n\cdot\lambda$ ⇒ constructive interference

$$\therefore \boxed{2d\sin\theta = n\cdot\lambda}$$

(1) ⇒ $n\cdot\lambda = 3\mu m\cdot\sin\theta$

Crystal :

invariant under translation : $T = u_1 a_1 + u_2 a_2 + u_3 a_3$

electron density : $n(x+a) = n(x)$ ⇒ periodicity allows us to treat this in fourier analysis

e.g. $n(x)$ is an a-periodic function in real space, we can expand it in fourier series :

$$n(x) = \sum_{p\neq 0} n_p \exp\left(i\cdot\underbrace{\frac{2\pi p}{a}}_{K}\cdot x\right)$$

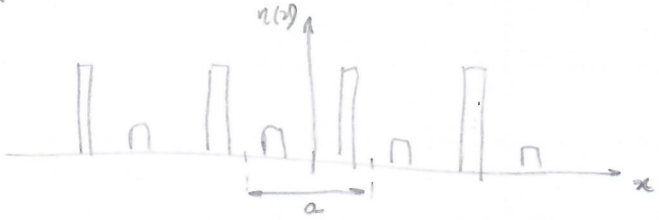
since $n(x+a) = n(x)$

$\Rightarrow K = \frac{2\pi}{a}p$

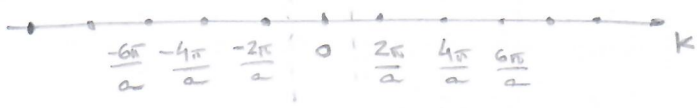
$\frac{2\pi}{a}p$ is a point of the reciprocal space (fourier space)

↳ these are the allowed terms in the fourier series.

real space



k-space (reciprocal space)



$\vec{K}$ is the reciprocal lattice vector.

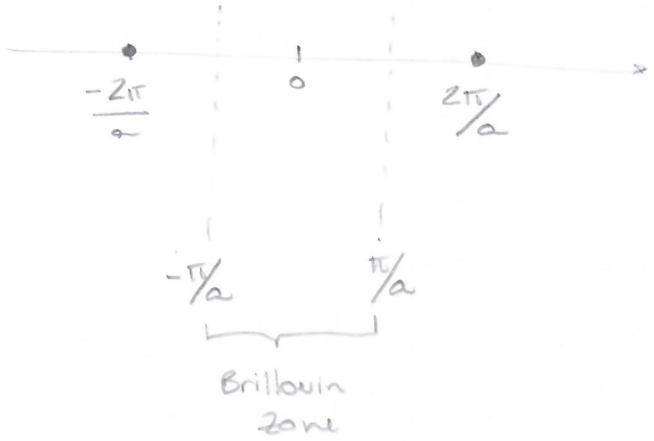
⇒ allowed points in reciprocal space (or components in the fourier series)

Reciprocal space

In 1D : $k \cdot a = p \cdot 2\pi$, in 3D : $\vec{r} \cdot \vec{G} = p \cdot 2\pi$

$$\begin{cases} \vec{T} = (a_1, a_2, a_3) \\ \vec{G} = (b_1, b_2, b_3) \end{cases} \Rightarrow \begin{cases} b_1 = 2\pi \dfrac{a_2 \times a_3}{a_1 \cdot a_2 \times a_3} \\ b_2 = 2\pi \cdot \dfrac{a_3 \times a_1}{a_1 \cdot a_2 \times a_3} \\ b_3 = 2\pi \dfrac{a_1 \times a_2}{a_1 \cdot a_2 \times a_3} \end{cases}$$

1D.



Bragg Law

extra light

$2L = 2d \sin\theta = n \cdot \lambda$

$\therefore \boxed{d \sim n \cdot \dfrac{\lambda}{2 \sin\theta}}$

diffraction from the reciprocal lattices

in CD : $d = 1.5\,\mu m$

λ : 400 – 700 nm

Schroedinger Equation:

⇒ allowed energy levels in a quantum mechanical system

⇒ respective wavefunctions: represent the probability of finding a particle in a given position

⇒ Good representation since Energy (E) and momentum (k) must be conserved.

$$\left[-\frac{\hbar^2}{2m^*} \nabla^2 + V(r) \right] \psi(r) = E(r)\,\psi(r) \qquad (1)$$

(∇^2: Laplacian)

Bloch theorem: if a potential $V(r)$ is periodic in real space, the solutions of (1) are of the form of a Bloch function:

$$\psi(r,k) = e^{j\vec{k}\cdot\vec{r}}\, u_b(r,k)$$

$\psi(r,k)$, $u_b(r,k)$ are both periodic in real space:

$$\psi(r+R,k) = \psi(r,k)$$

$$e^{j\vec{k}(\vec{r}+\vec{R})}\, u_b(r+R,k) = e^{j\vec{k}\vec{r}}\, u_b(r,k)$$

$$= u_b(r,k)$$

$$\Rightarrow e^{j\vec{k}\cdot\vec{R}} = 1 \Rightarrow \boxed{\vec{k}\cdot\vec{R} = n\cdot 2\pi}$$

⇒ only $\vec{k}$ that satisfy this condition are allowed. ⇒ Defines the Brillouin zone in reciprocal space

⇒ Function is also periodic in k-space ⇒ $K = K + \vec{G}$

(*) in 1D: if a function is periodic $R = a$ the reciprocal vector is periodic of $G = \frac{2\pi}{a}$ ⇒ $[-\pi/a, \pi/a]$ are edges of the Brillouin zone.

in 3D: $k_x = n\cdot\frac{\pi}{L_x}$, $k_y = m\frac{\pi}{L_y}$, $k_z = l\cdot\frac{\pi}{L_z}$ ⇒ quantization of k in k-space

(*) the energy $E(k) = E(k+G)$ is also periodic.

---

for electrons

$\vec{k}$ gives the direction of where the wavefunction is propagating

momentum: $\vec{P} = \hbar\vec{k}$ (classically: $\vec{P} = m\cdot\vec{v}$ and $E = \frac{m^2v^2}{2m} = \frac{1}{2}m\vec{v}^2$)

energy: $E = \frac{\hbar^2k^2}{2m_e^*} = \frac{|\vec{P}|^2}{2m_e^*}$