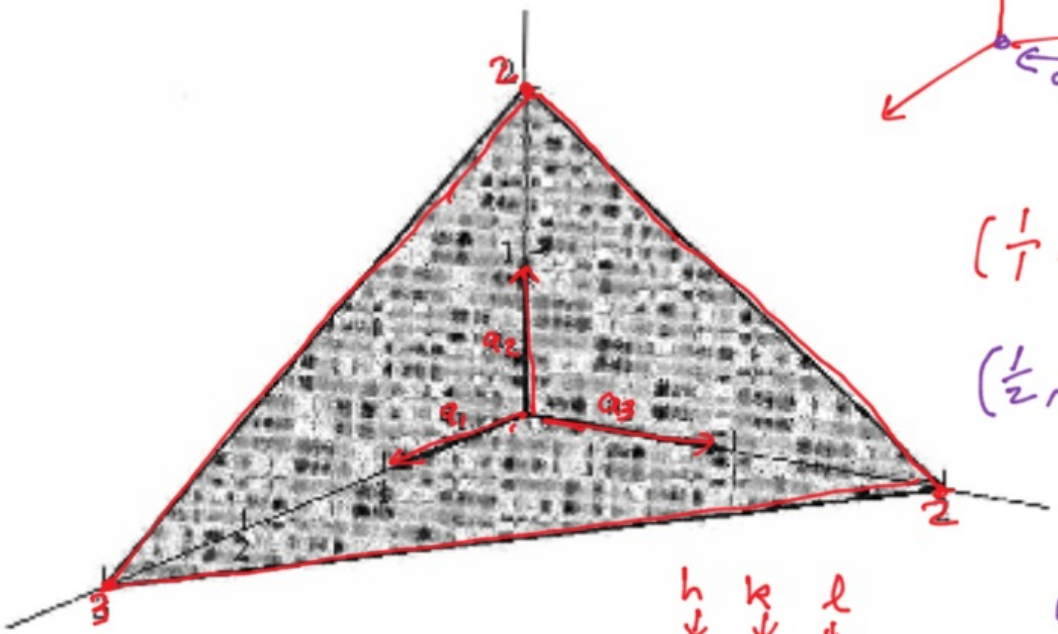
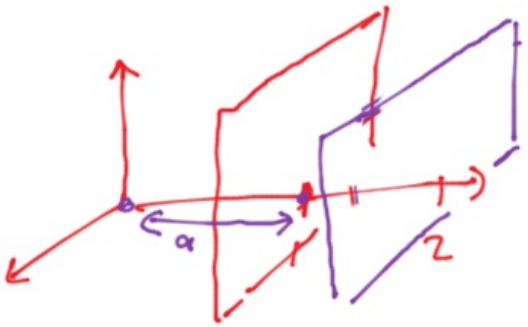
LATTICE PLANES: Miller indices (h, k, l)





$\left(\frac{1}{1}, \frac{1}{\infty}, \frac{1}{\infty}\right) = (1, 0, 0)$

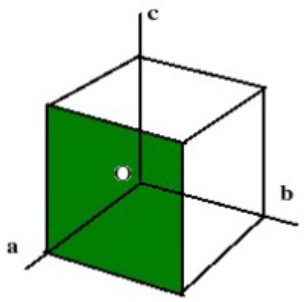
$\left(\frac{1}{2}, 0, 0\right)$ $(1, 0, 0)$

$\left(\frac{1}{3}, \frac{1}{2}, \frac{1}{2}\right) \rightarrow \begin{matrix} h & k & l \\ \downarrow & \downarrow & \downarrow \\ (2, & 3, & 3) \end{matrix}$

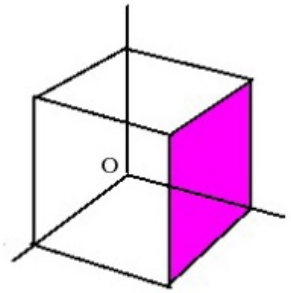
$d_{hkl} = a$

$d_{hkl} = \frac{a}{\sqrt{h^2 + k^2}}$

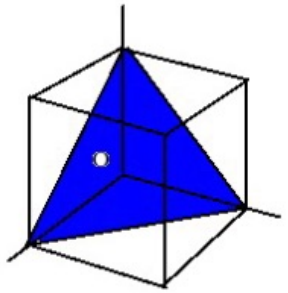
LATTICE PLANES: Miller indices



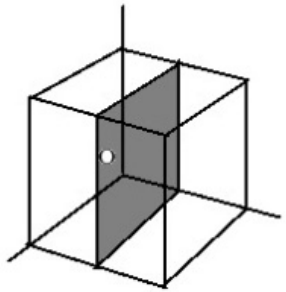
(1 0 0)



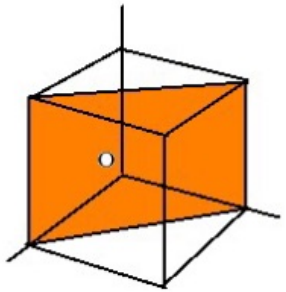
(0 1 0)



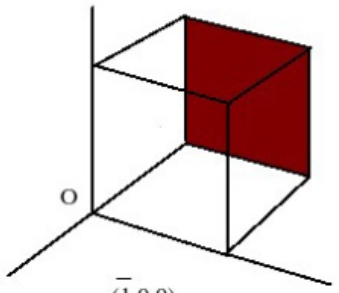
(1 1 1)



(0 2 0)

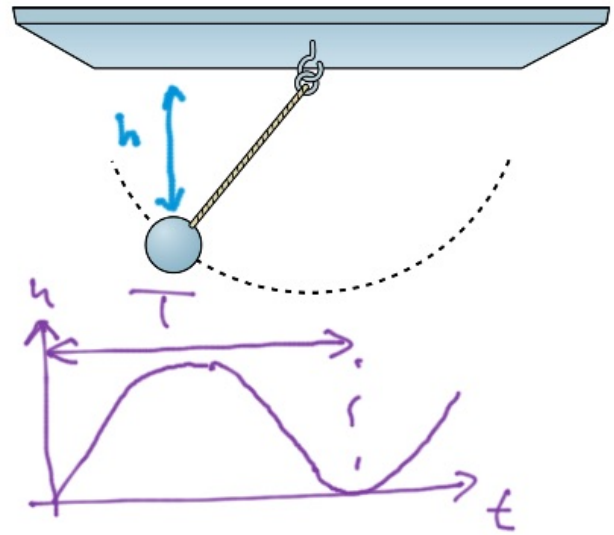


(1 1 0)



($\bar{1}$ 0 0)

REAL TIME:

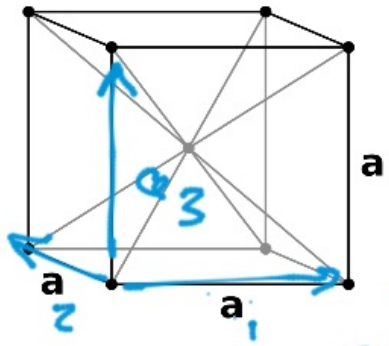


Reciprocal time

Angular frequency

$$\omega = \frac{2\pi}{T} \quad [1/s]$$

REAL SPACE:



Units

[Å]

Dimension

3

RECIPROCAL SPACE:

Units

$\frac{2\pi}{a}$ $[\AA^{-1}]$

Dimensions

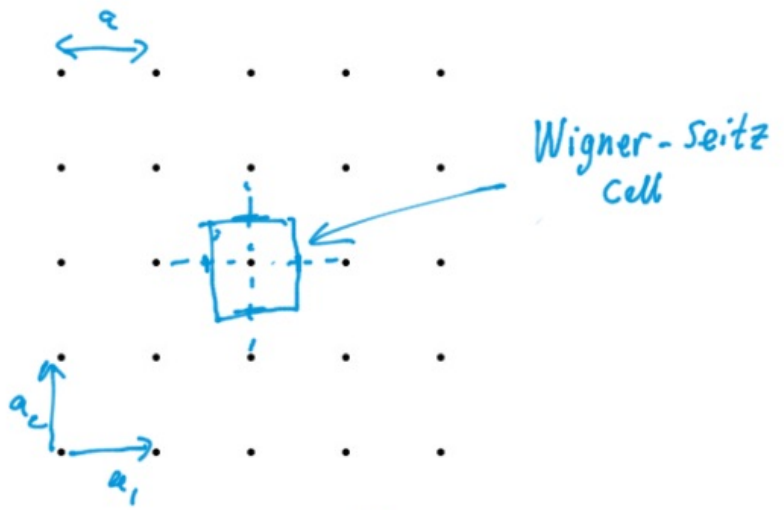
3

$$\vec{r} = \mu_1 \vec{a}_1 + \mu_2 \vec{a}_2 + \mu_3 \vec{a}_3$$

$$\vec{\tilde{r}} = \tilde{\mu}_1 \vec{b}_1 + \tilde{\mu}_2 \vec{b}_2 + \tilde{\mu}_3 \vec{b}_3$$

μ_i = integer numbers

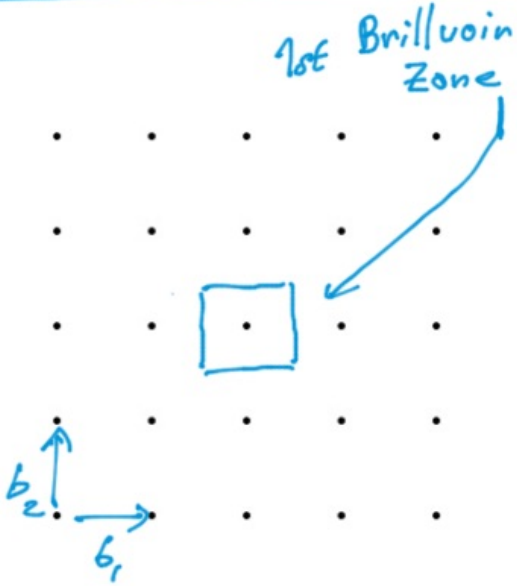
REAL SPACE SQUARE LATTICE:



$a_1 = (1, 0)$

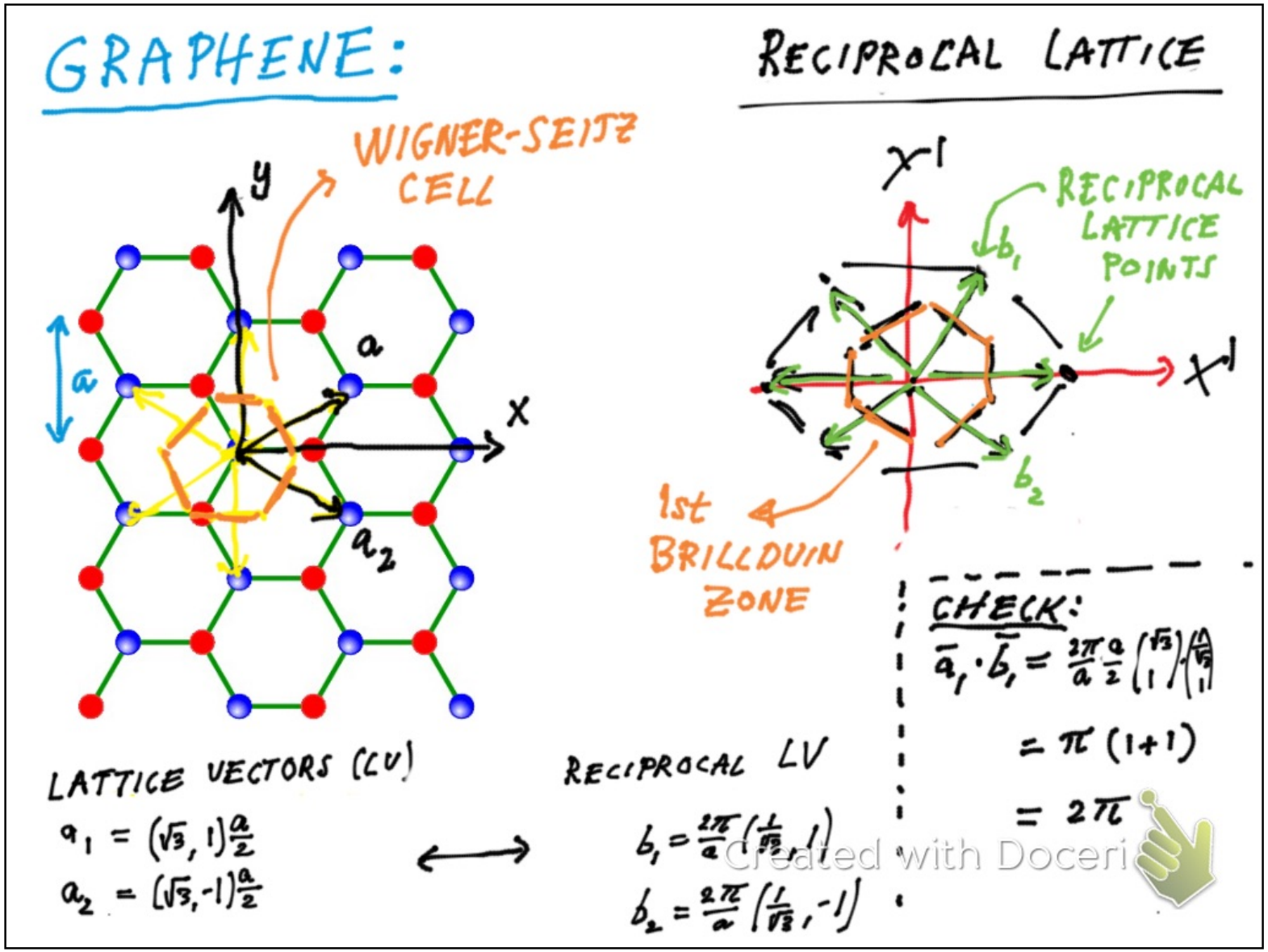
$a_2 = (0, 1)$

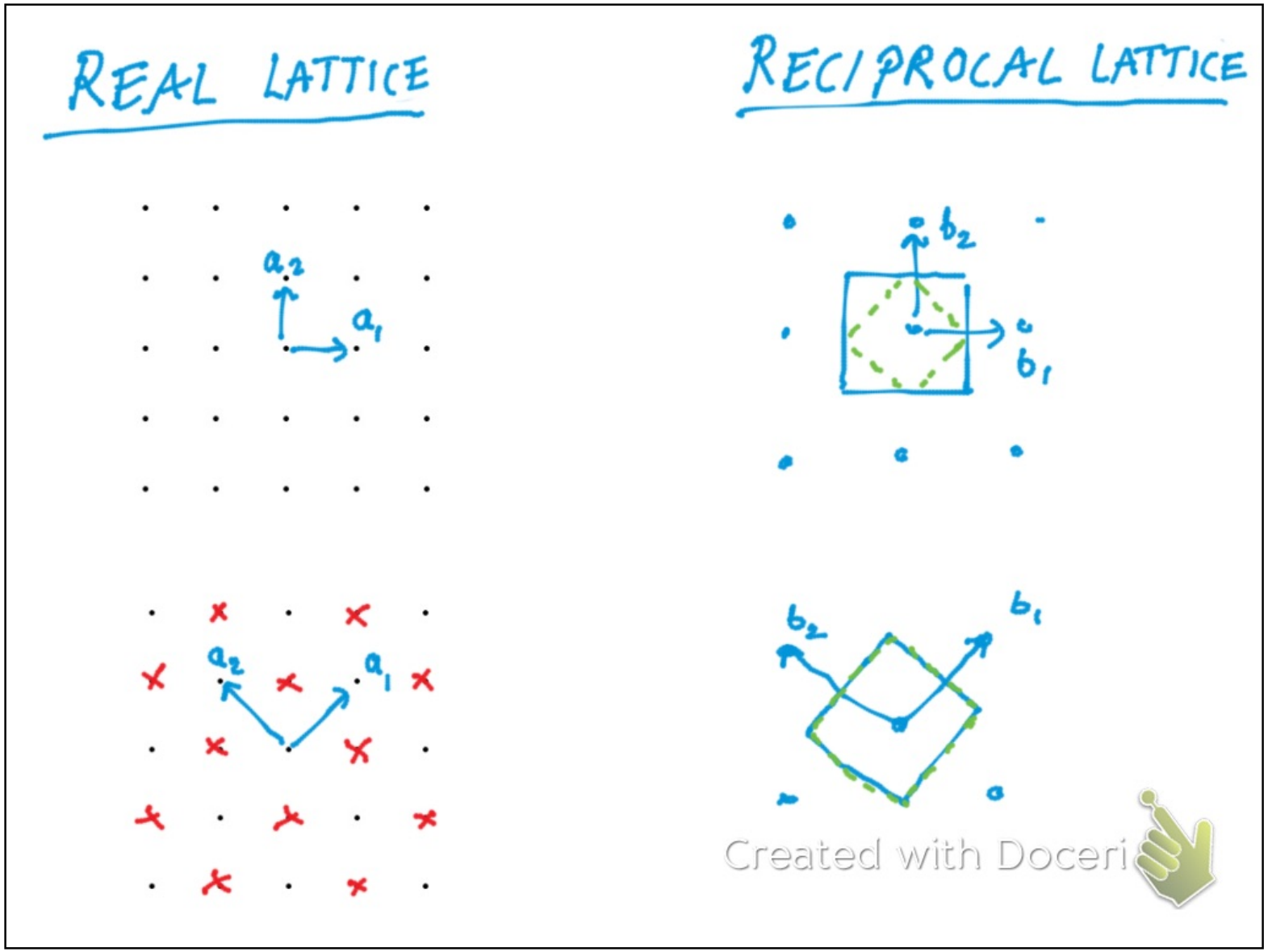
RECIPROCAL LATTICE:



$b_1 = \frac{2\pi}{a}(1, 0)$

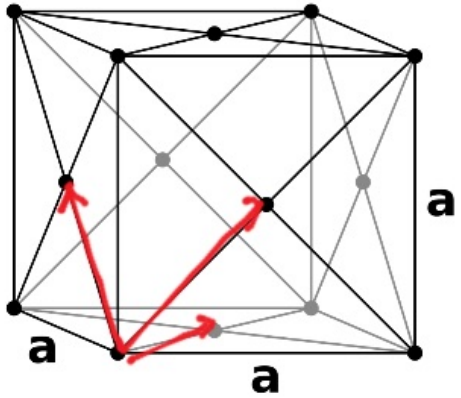
$b_2 = \frac{2\pi}{a}(0, 1)$


GRAPHENE:
WIGNER-SEITZ CELL
y
x
a
a
a_2
LATTICE VECTORS (LV)
$a_1 = (\sqrt{3}, 1)\frac{a}{2}$
$a_2 = (\sqrt{3}, -1)\frac{a}{2}$
RECIPROCAL LV
$b_1 = \frac{2\pi}{a}(\frac{1}{\sqrt{3}}, 1)$
$b_2 = \frac{2\pi}{a}(\frac{1}{\sqrt{3}}, -1)$
RECIPROCAL LATTICE
x^1
x^1
RECIPROCAL LATTICE POINTS
b_1
b_2
1st BRILLOUIN ZONE
CHECK:
$\bar{a}_1 \cdot \bar{b}_1 = \frac{2\pi}{a}\frac{a}{2}\begin{pmatrix}\sqrt{3}\\1\end{pmatrix}\begin{pmatrix}\frac{1}{\sqrt{3}}\\1\end{pmatrix}$
$= \pi(1+1)$
$= 2\pi$
Created with Doceri


REAL LATTICE
RECIPROCAL LATTICE
a_2
a_1
b_2
b_1
Created with Doceri

LATTICE VECTORS:

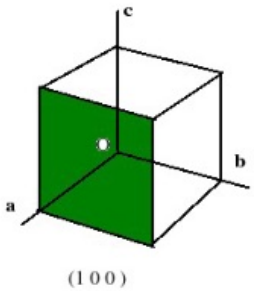
RECIPROCAL LATTICE VECTORS



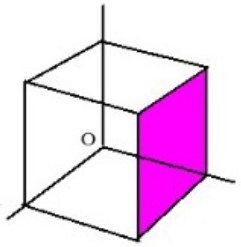
EXERCISE SHEET 2

EXERCISE 2

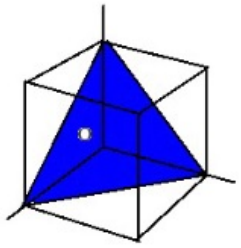
EXERCISE



(1 0 0)

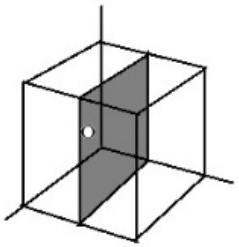


(0 1 0)

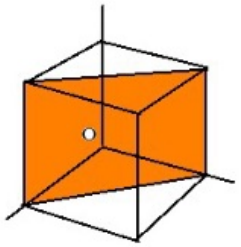


(1 1 1)

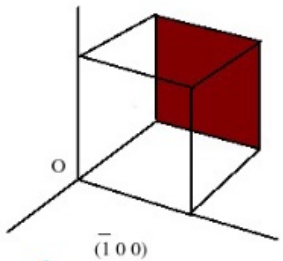
(hkl)



(0 2 0)



(1 1 0)



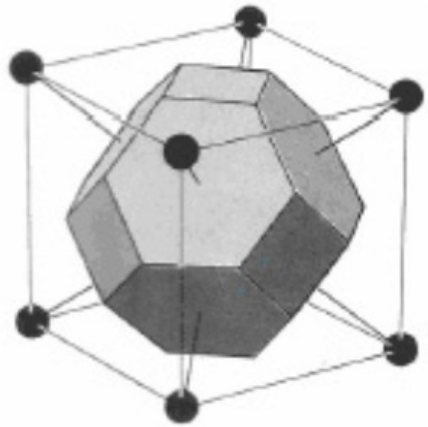
($\bar{1}$ 0 0)

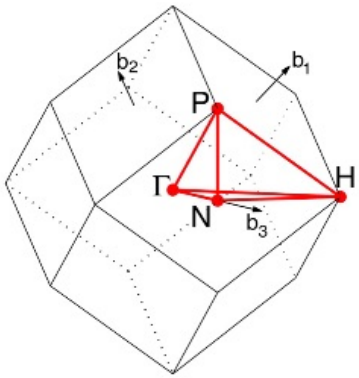
Reciprocal vector: $\vec{G} = h\vec{b}_1 + k\vec{b}_2 + l\vec{b}_3$

$\vec{G} \perp$ to lattice plane (hkl)

WIGNER-SEITZ CELL ⟷ BRILLOUIN ZONE

BCC

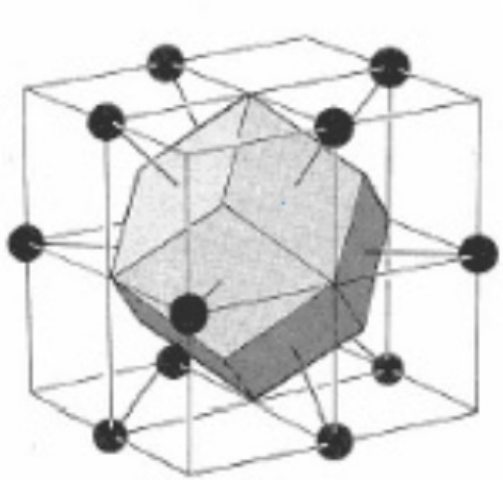


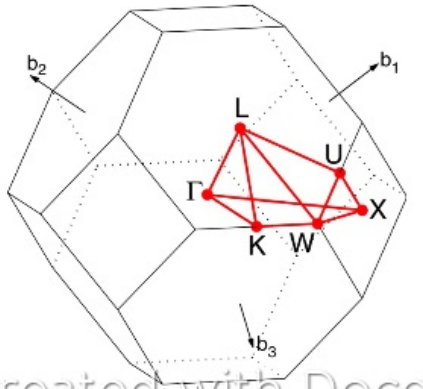


BCC path: Γ-H-N-Γ-P-H|P-N

[Setyawan & Curtarolo, DOI: 10.1016/j.commatsci.2010.05.010]

FCC

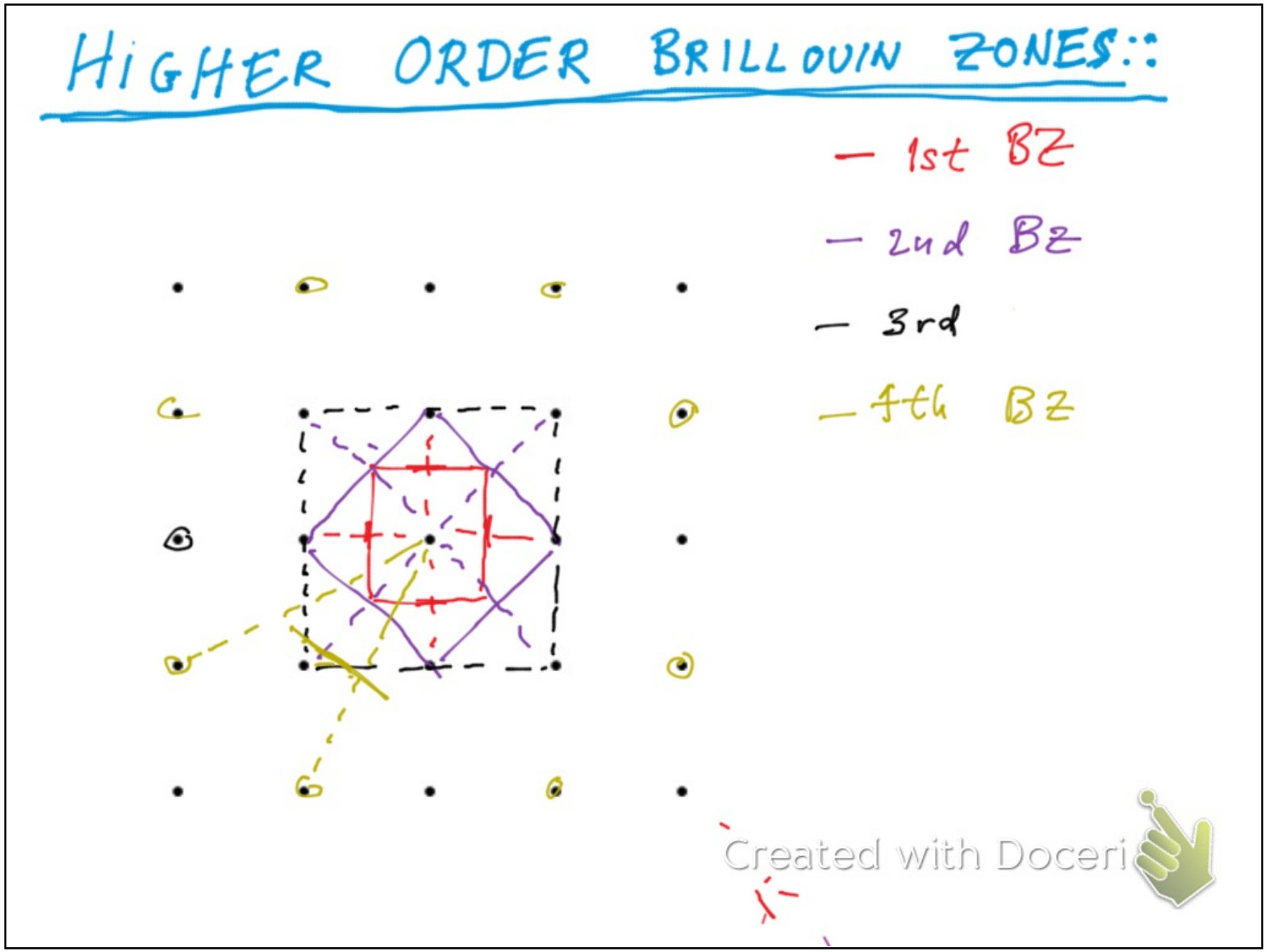




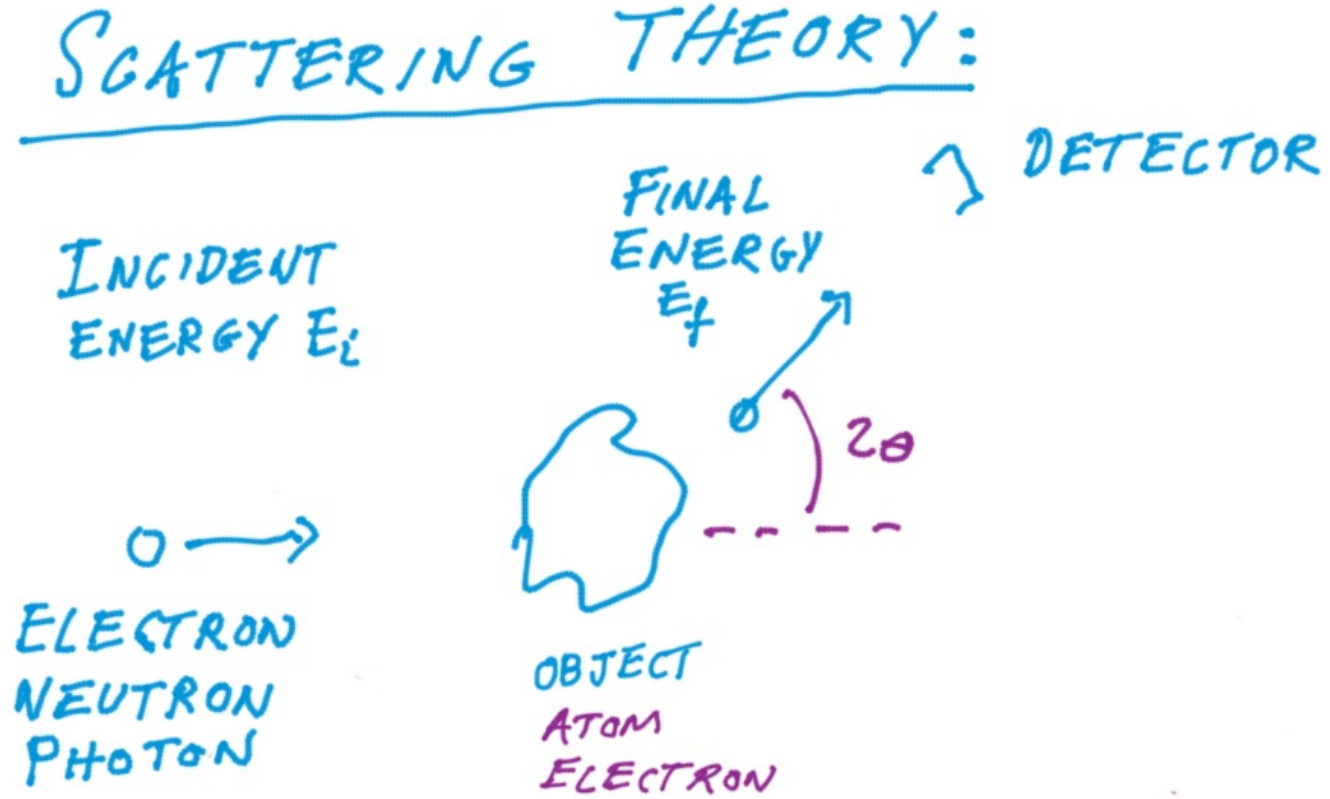
FCC path: Γ-X-W-K-Γ-L-U-W-L-K|U-X

[Setyawan & Curtarolo, DOI: 10.1016/j.commatsci.2010.05.010]

HIGHER ORDER BRILLOUIN ZONES::



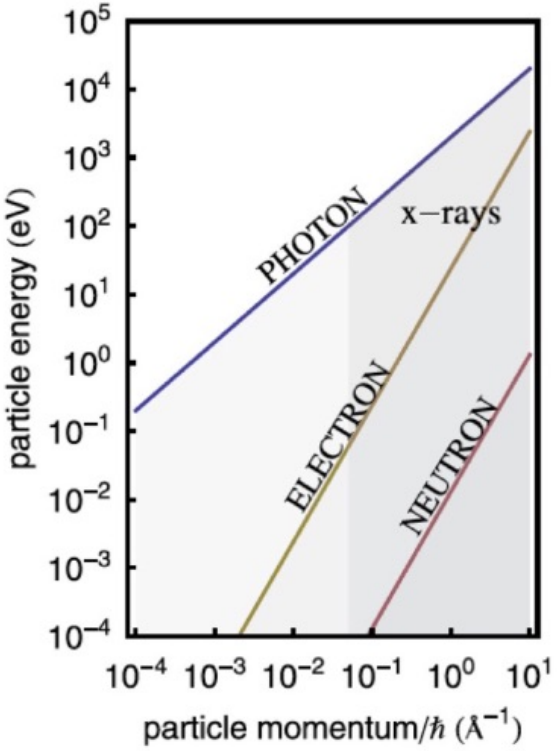
SCATTERING THEORY:



ELASTIC SCATTERING MEANS:

$$E_i = E_f$$

DISPERSION RELATION:



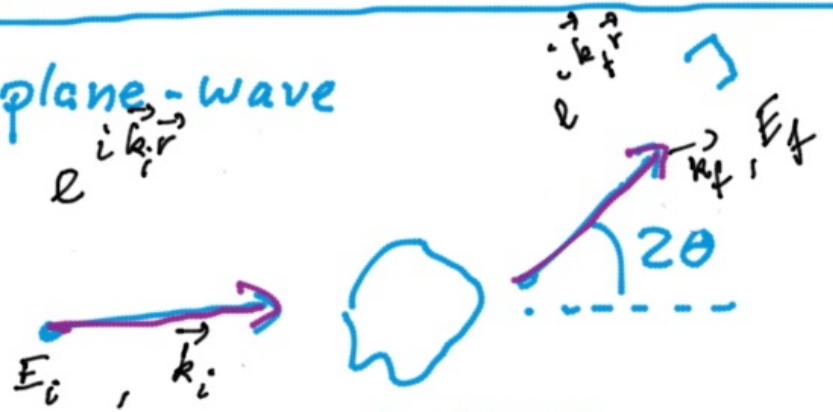
Neutron or Electron

$$E = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m}$$

Photon

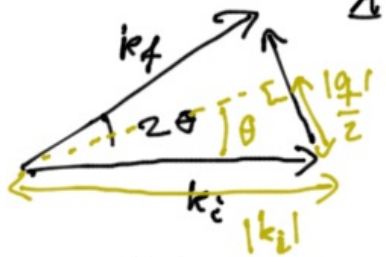
$$E = hck$$

SCATTERING TRIANGLE:



WE CONSIDER ELASTIC SCATTERING: $E_i = E_f$

$$\Delta\vec{k} = \vec{q} = \vec{k}_f - \vec{k}_i \quad \text{(scattering vector)}$$



$$|q| = f(\theta) = 2|k_i|\sin\theta$$

$$|k_i| = |k_f|$$