

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

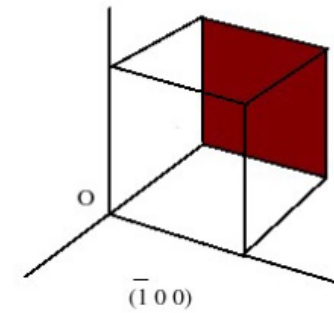
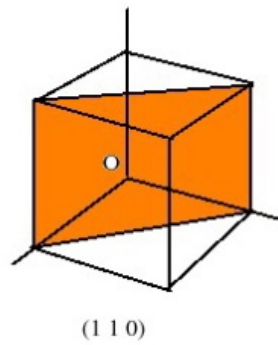
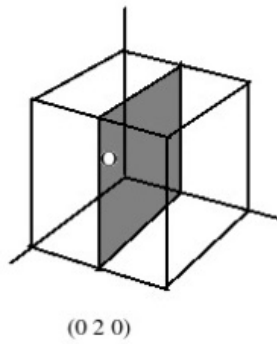
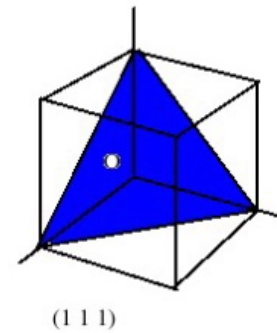
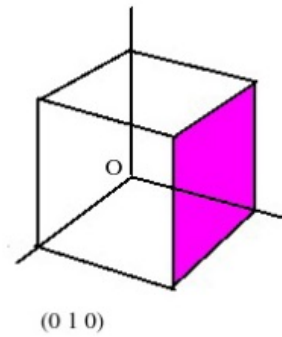
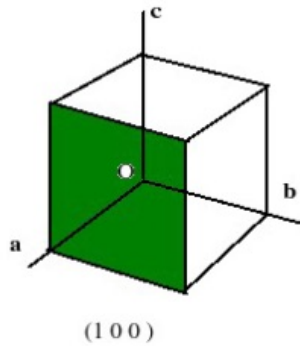
$(\frac{1}{3}, \frac{1}{2}, \frac{1}{2}) \rightarrow \begin{matrix} h & k & l \\ \downarrow & \downarrow & \downarrow \\ 2 & 3 & 3 \end{matrix}$

$(\frac{1}{1}, \frac{1}{\infty}, \frac{1}{\infty}) = (1, 0, 0)$   
 $(\frac{1}{2}, 0, 0) \quad (1, 0, 0)$

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

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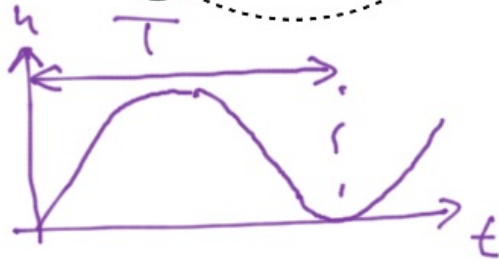
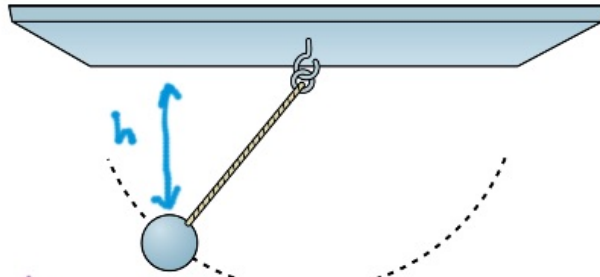
# LATTICE PLANES: Miller indices



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## REAL TIME:



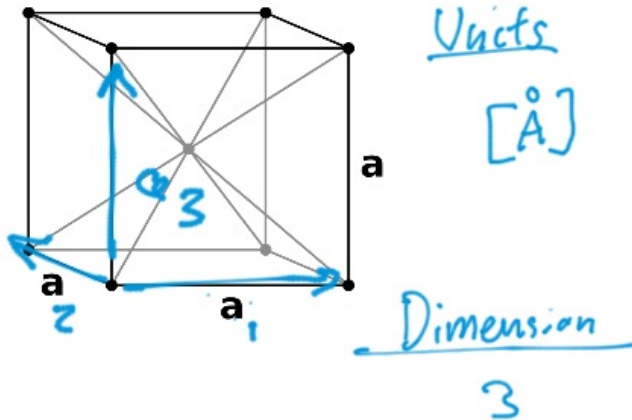
Reciprocal time

Angular frequency

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

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## REAL SPACE:



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

$\mu_i = \text{integer numbers}$

## RECIPROCAL SPACE:

Units  
 $\frac{2\pi}{a}$  [Å<sup>-1</sup>]

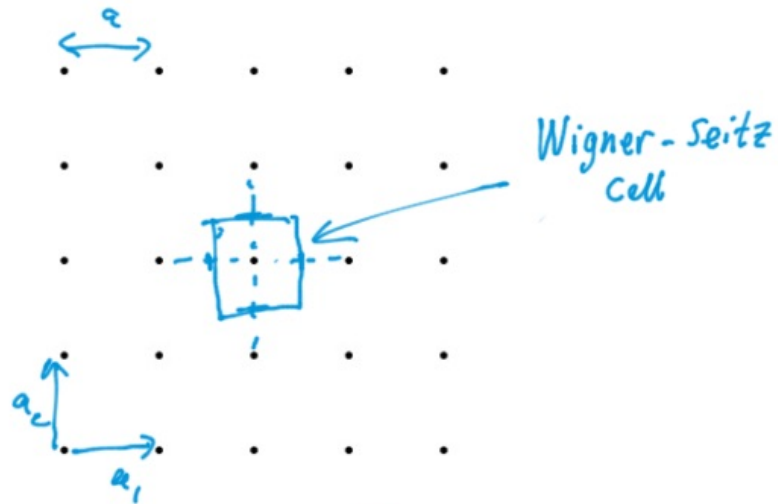
Dimensions  
3

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

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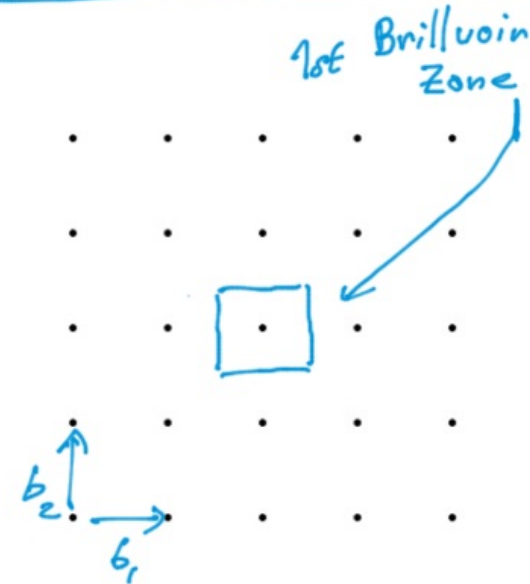
## REAL SPACE SQUARE LATTICE:



$$a_1 = (1, 0)$$

$$a_2 = (0, 1)$$

## RECIPROCAL LATTICE:



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

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

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## GRAPHENE:

WIGNER-SEITZ CELL

LATTICE VECTORS (LV)

$$a_1 = \left(\sqrt{3}, 1\right) \frac{a}{2}$$

$$a_2 = \left(\sqrt{3}, -1\right) \frac{a}{2}$$

## RECIPROCAL LATTICE

RECIPROCAL LATTICE POINTS

1st BRILLUIN ZONE

RECIPROCAL LV

$$b_1 = \frac{2\pi}{a} \left(\frac{1}{\sqrt{3}}, 1\right)$$

$$b_2 = \frac{2\pi}{a} \left(\frac{1}{\sqrt{3}}, -1\right)$$

**CHECK:**

$$\vec{a}_1 \cdot \vec{b}_1 = \frac{2\pi a}{a} \frac{1}{2} \begin{pmatrix} \sqrt{3} \\ 1 \end{pmatrix} \cdot \begin{pmatrix} 1/\sqrt{3} \\ 1 \end{pmatrix}$$

$$= \pi (1+1)$$

$$= 2\pi$$

# REAL LATTICE



# RECIPROCAL LATTICE

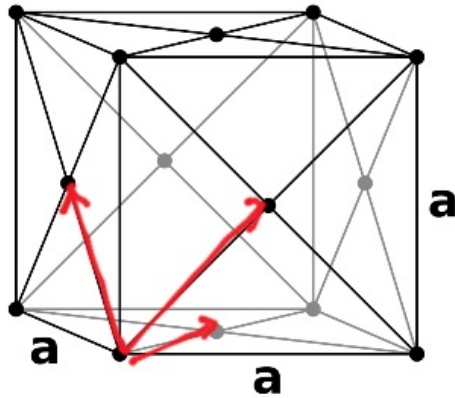


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LATTICE VECTORS:

RECIPROCAL LATTICE VECTORS

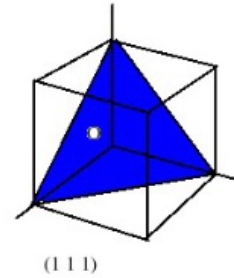
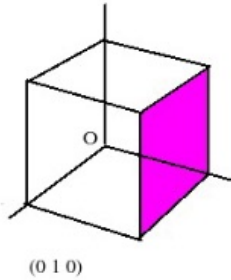
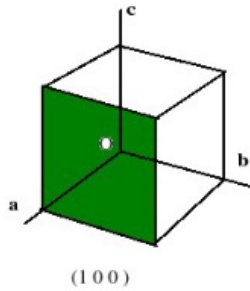


EXERCISE SHEET 2  
EXERCISE 2

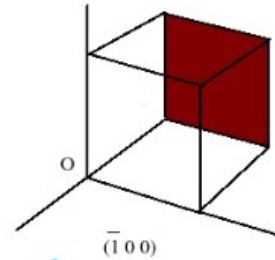
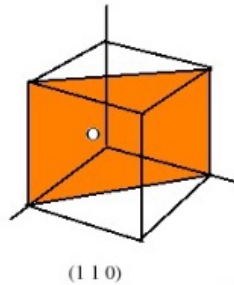
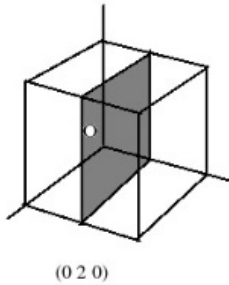
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## EXERCISE:



(hkl)



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

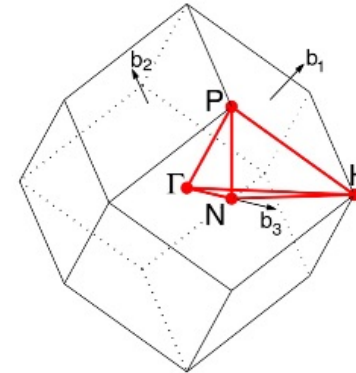
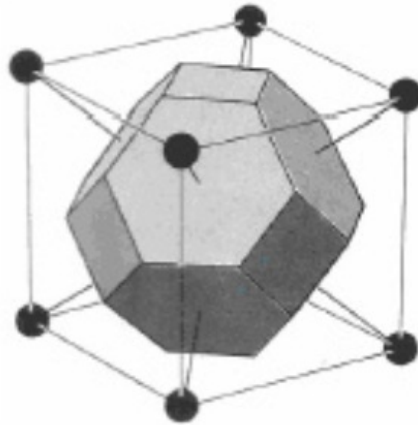
$\vec{G} \perp$  to lattice plane (hkl)

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# WIGNER-SEITZ CELL ↔ BRILLOUIN ZONE

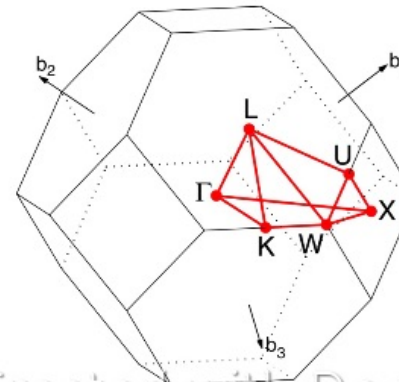
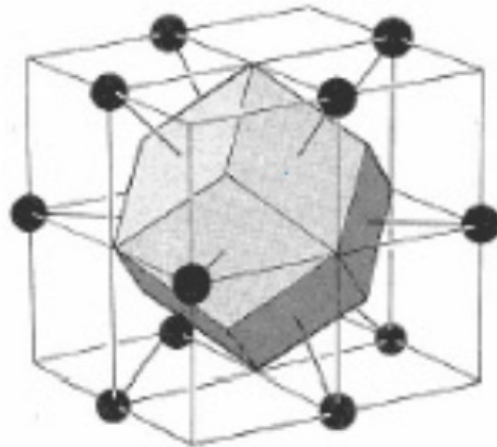
BCC



BCC path:  $\Gamma$ -H-N- $\Gamma$ -P-H|P-N

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

FCC



FCC path:  $\Gamma$ -X-W-K- $\Gamma$ -L-U-W-L-K|U-X

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


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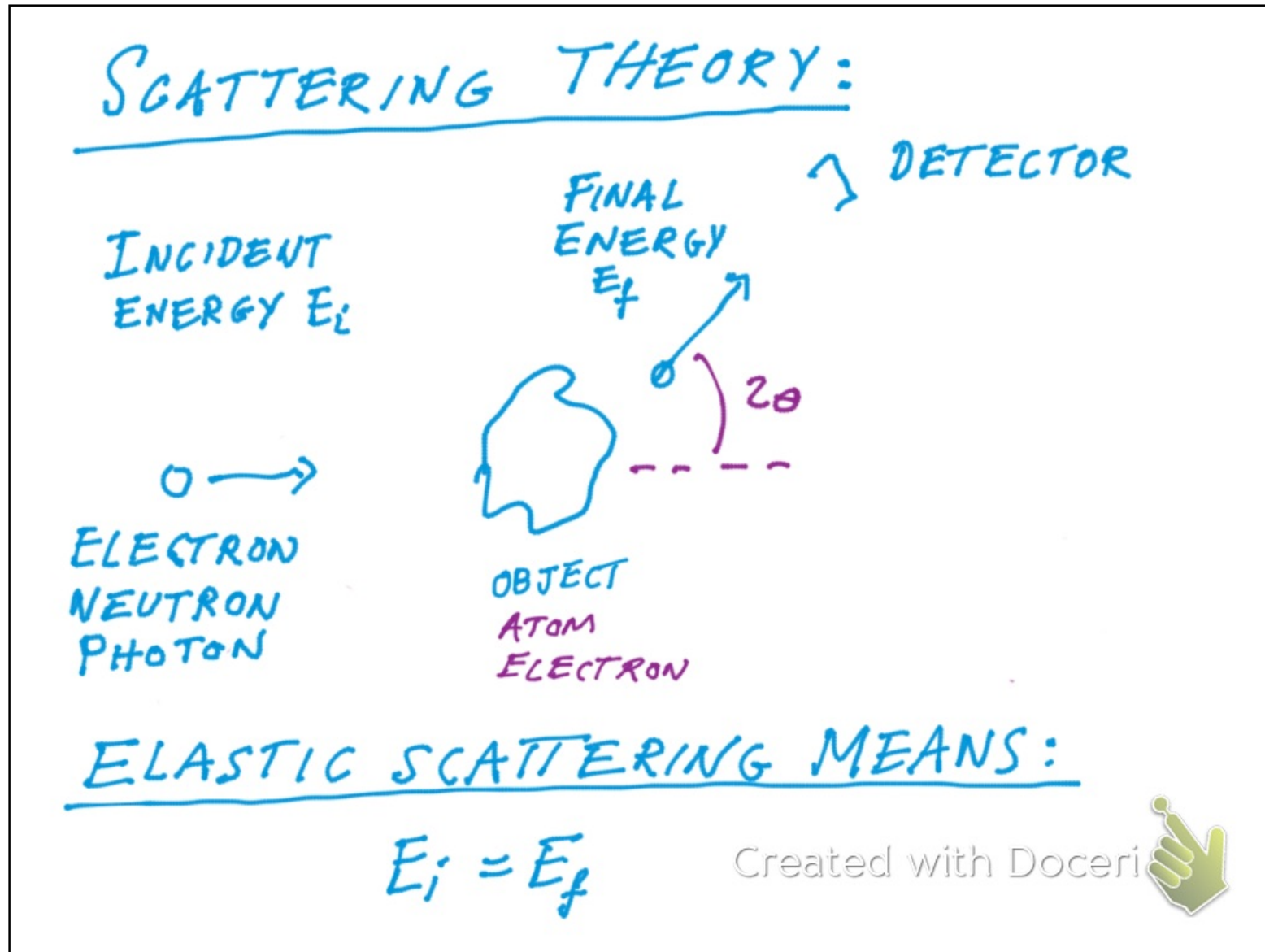


# HIGHER ORDER BRILLOUIN ZONES::

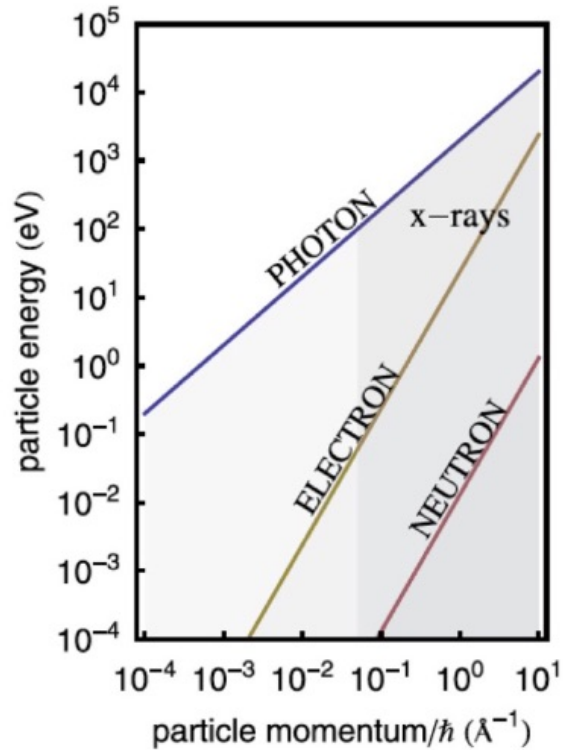
- 1st BZ
- 2nd BZ
- 3rd
- 4th BZ

The diagram illustrates the construction of higher-order Brillouin zones in a 2D square lattice. A central lattice point is surrounded by four other points. The first Brillouin zone (BZ) is a red square. The second BZ is a purple square rotated 45 degrees. The third BZ is a black dashed square. The fourth BZ is a yellow dashed square. A green hand icon is pointing to the diagram.

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## DISPERSION RELATION:



Neutron or Electron

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

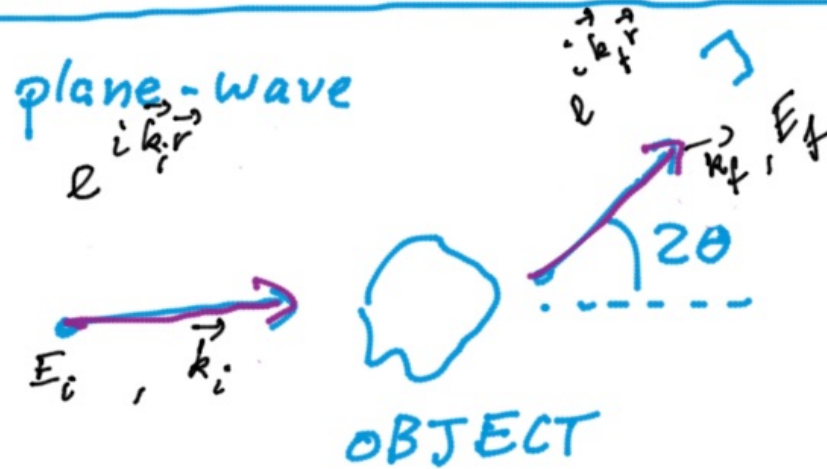
Photon

$$E = \hbar c k$$

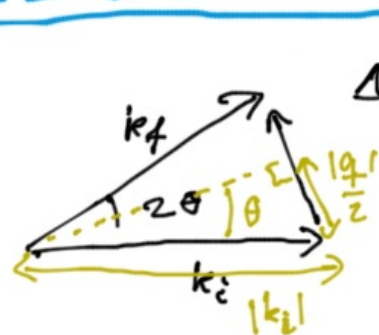
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# SCATTERING TRIANGLE:



WE CONSIDER ELASTIC SCATTERING:  $E_i = E_f$



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

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

$$|k_i| = |k_f|$$

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