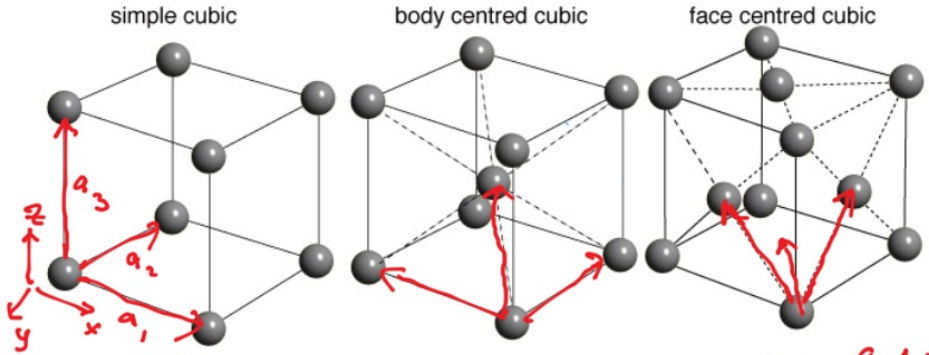
CRYSTAL LATTICE VECTORS:

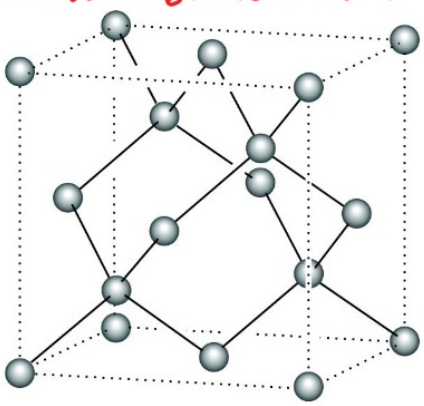
$LATTICE = BASIS + u_1\vec{a}_1 + u_2\vec{a}_2 + u_3\vec{a}_3$ with u_1, u_2, u_3 = integers

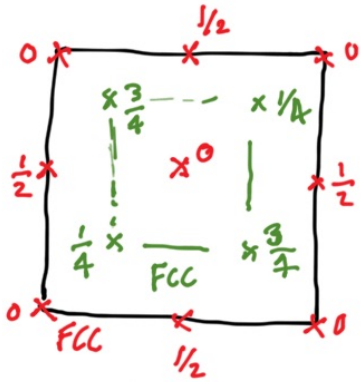


simple cubic	body centred cubic	face centred cubic
$a_1 = a\,(100)$	$a_1 = a\,(100)$	$a_1 = \frac{a}{2}(110)$
$a_2 = a\,(010)$	$a_2 = a\,(010)$	$a_2 = \frac{a}{2}(011)$
$a_3 = a\,(001)$	$a_3 = \frac{a}{2}(111)$	$a_3 = \frac{a}{2}(101)$
Basis = {000}	Basis = {000}	Basis = {000}

CRYSTAL LATTICE VECTORS:

$LATTICE = BASIS + u_1\vec{a}_1 + u_2\vec{a}_2 + u_3\vec{a}_3$ with u_1, u_2, u_3 = integers





LATTICE VECTORS

$a_1 = \frac{a}{2}(110)$

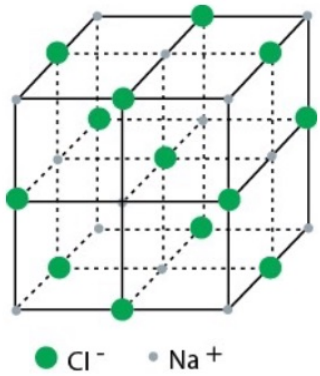
$a_2 = \frac{a}{2}(011)$

$a_3 = \frac{a}{2}(101)$

$BASIS = \{(000), (\frac{1}{4}\frac{1}{4}\frac{1}{4})a\}$

CRYSTAL LATTICE VECTORS:

LATTICE = BASIS + $u_1\vec{a}_1 + u_2\vec{a}_2 + u_3\vec{a}_3$ with u_1, u_2, u_3 = integers



LATTICE VECTORS

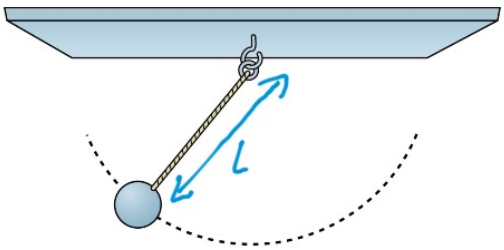
$a_1 = \frac{a}{2}(110)$

$a_2 = \frac{a}{2}(011)$

$a_3 = \frac{a}{2}(101)$

BASIS = $\{(000), (\frac{1}{2}\frac{1}{2}\frac{1}{2})a\}$

Reciprocal time



FREQUENCY f $[hz] = [s^{-1}]$

$$T = \frac{1}{f} = 2\pi\sqrt{\frac{L}{g}}$$

RECIPROCAL LATTICE VECTORS

$$b_1 = 2\pi\frac{a_2 \times a_3}{a_1 \cdot a_2 \times a_3}$$

$$b_2 = 2\pi\frac{a_1 \times a_3}{a_2 \cdot a_1 \times a_3}$$

$$b_3 = 2\pi\frac{a_1 \times a_2}{a_3 \cdot a_1 \times a_2}$$

$a_i \cdot b_j = 2\pi\delta_{ij}$

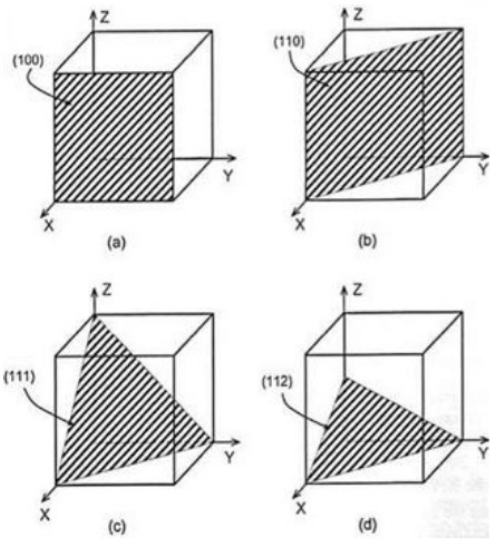
RECIPROCAL LATTICE Units

$[2\pi/a]$

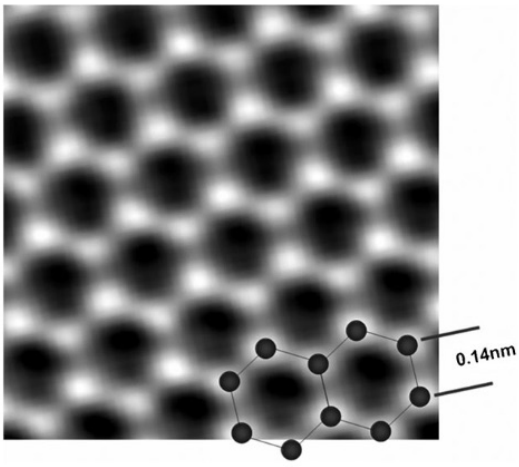
RECIPROCAL LATTICE SPACE

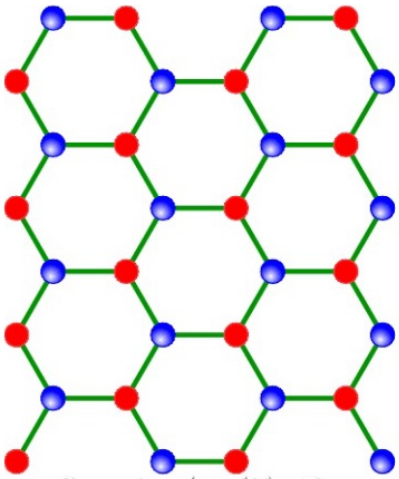
$\vec{G} = h\vec{b}_1 + k\vec{b}_2 + l\vec{b}_3$

MILLER INDICES:

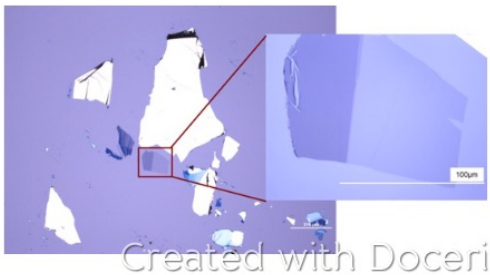


GRAPHENE : A SHEET OF CARBON



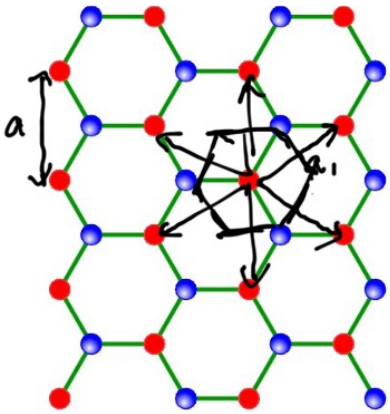


MAKING OF GRAPHENE:



GRAPHENE:

BASIS = $\{(0,0); (-\frac{1}{\sqrt{3}}, 0)\}$

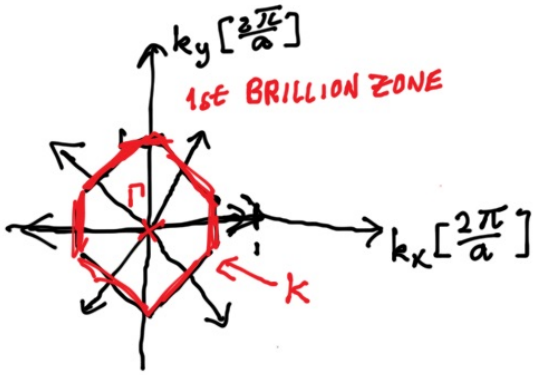


Lattice vectors

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

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

RECIPROCAL SPACE

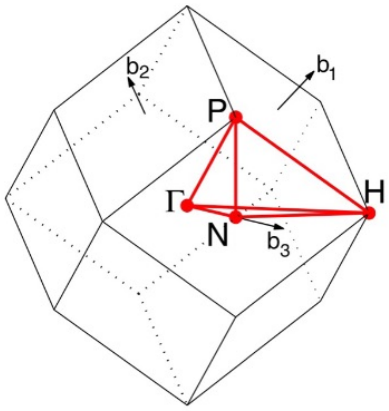


Reciprocal lattice vectors

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

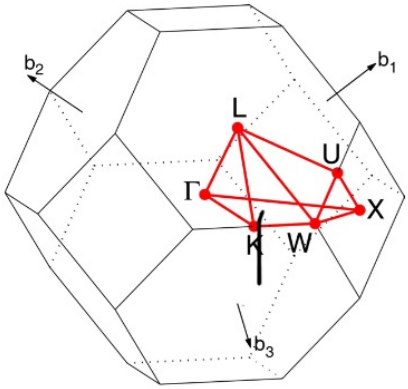
$b_2 = \frac{2\pi}{a}(\frac{1}{\sqrt{3}}, -1)$

BRILLOUIN ZONES



BCC path: Γ-H-N-Γ-P-H|P-N

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



FCC path: Γ-X-W-K-Γ-L-U-W-L-K|U-X

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

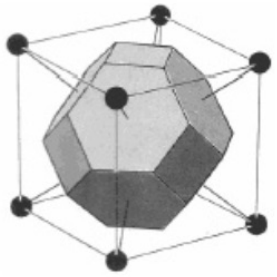
WIGNER-SEITZ CELL vs BRILLOUN ZONE

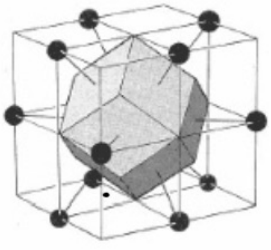
BCC

FCC

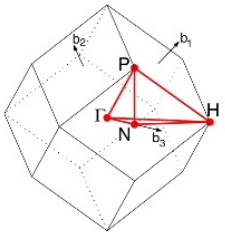
REAL SPACE

WIGNER SEITZ CELL





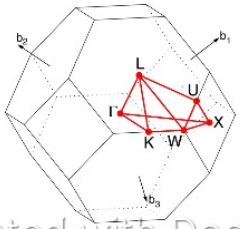
Reciprocal space



BCC path: Γ-H-N-Γ-P-H|P-N

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

Brillouin ZONE

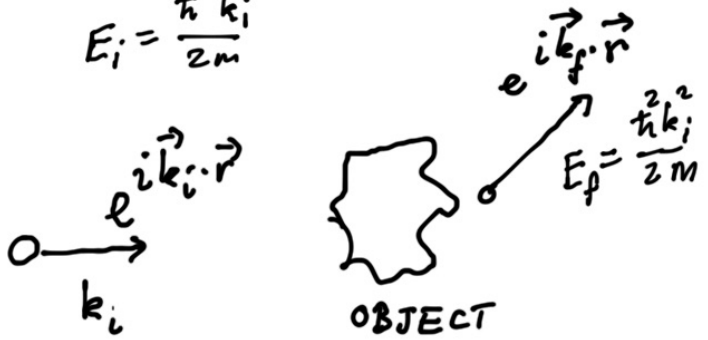


FCC path: Γ-X-W-K-Γ-L-U-W-L-K|U-X

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

SCATTERING: SINGLE OBJECT

$E_i = \frac{\hbar^2 k_i^2}{2m}$

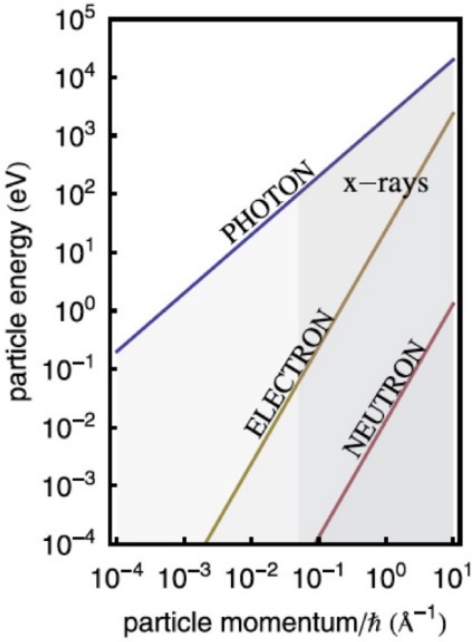


ELECTRON
NEUTRON
PHOTON

ATOM
ELECTRON

Elastic scattering means that: $E_i = E_f$

DISPERSION:



ELECTRONS & NEUTRONS

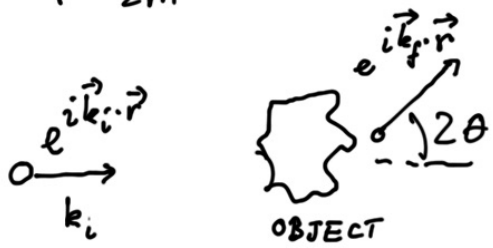
$$E = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m} = \frac{h}{2m\lambda^2}$$

PHOTONS:

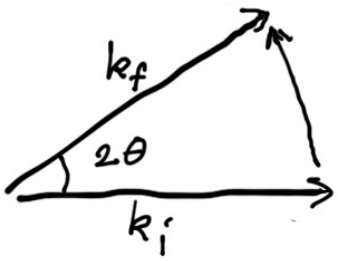
$$E = \hbar c k = \frac{hc}{\lambda}$$

SCATTERING TRIANGLE:

$E_i = \frac{\hbar^2 k_i^2}{2m}$ $\quad E_f = \frac{\hbar^2 k_f^2}{2m}$



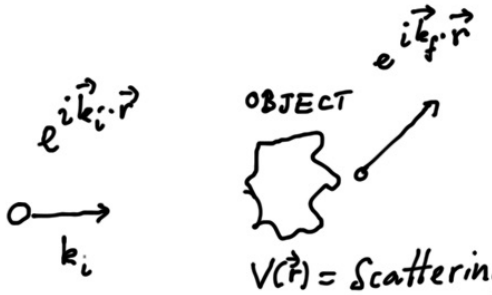
We consider the case: $E_i = E_f$



$\Delta k = \vec{q} = \vec{k}_f - \vec{k}_i$

$q = 2k_i \cdot \sin(\theta)$

SCATTERING PROBABILITY:



$V(\vec{r})$ = Scattering potential