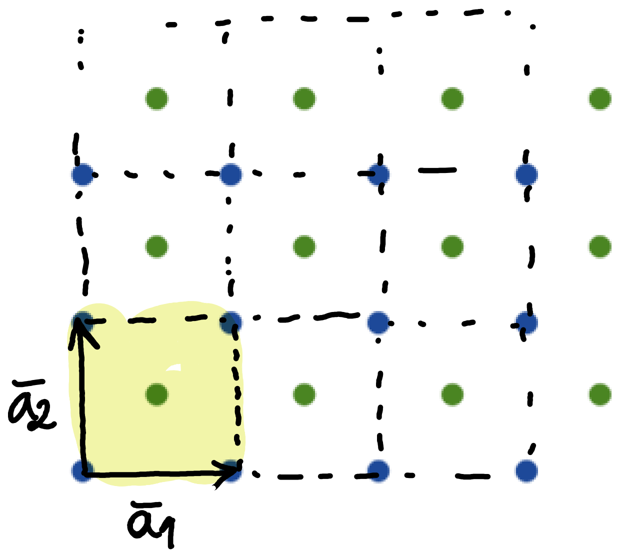
Reciprocal Lattice

Recap



Basis ● (0,0)
● (½,½)

CRYSTAL = LATTICE + BASIS

translation symmetry

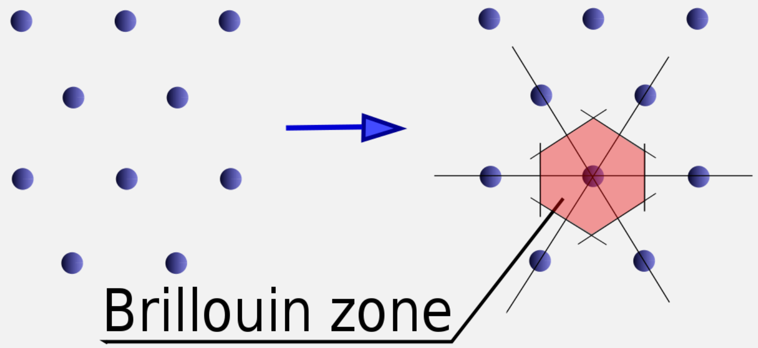
$\vec{r}' = \vec{r} + \vec{T} = \vec{r} + n_1\bar{a}_1 + n_2\bar{a}_2 + n_3\bar{a}_3$

$\bar{a}_i$: primitive lattice vectors

n_i : arbitrary integers

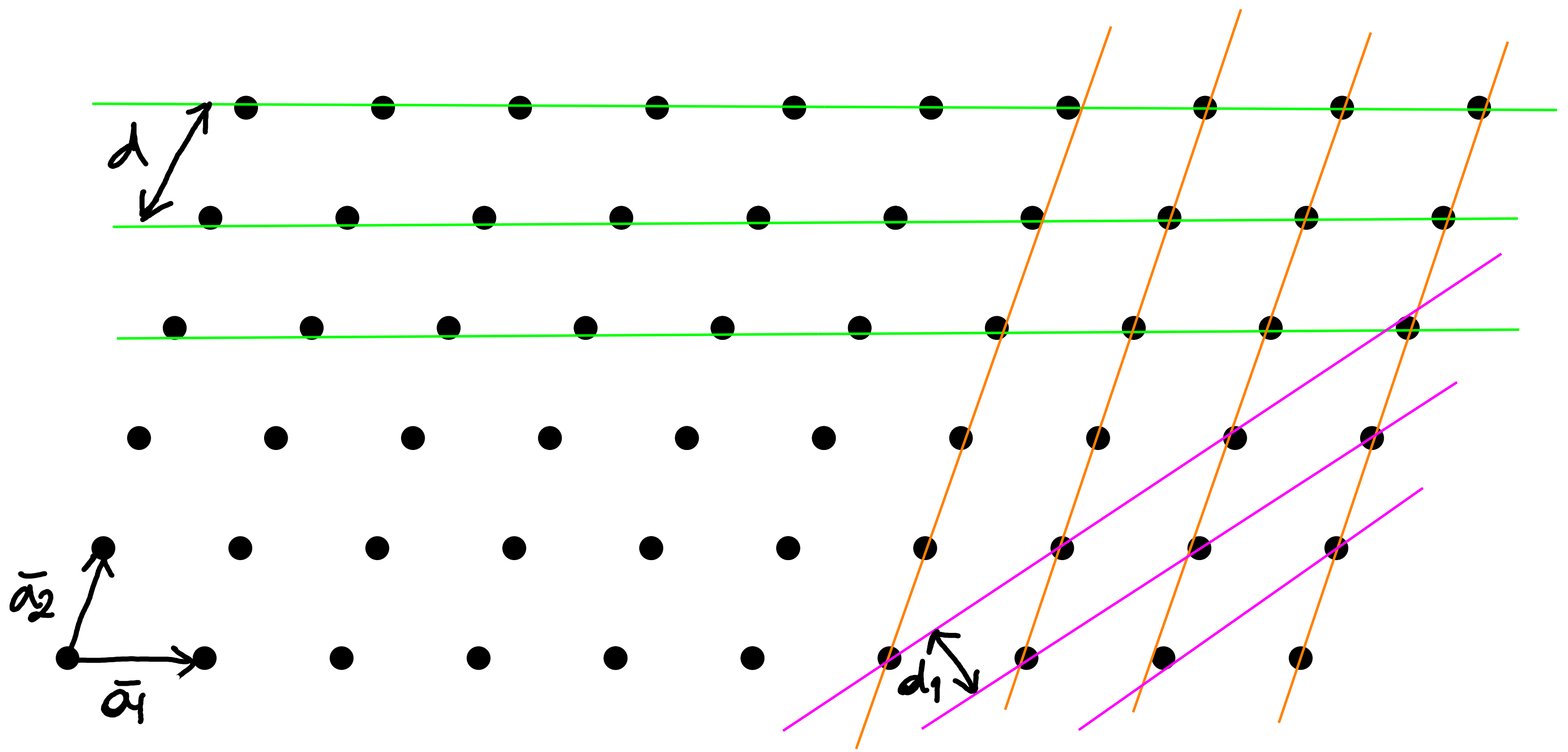
Learning outcomes of today

- Lattice planes
- Introduction to diffraction: Bragg Law
- Reciprocal Lattice



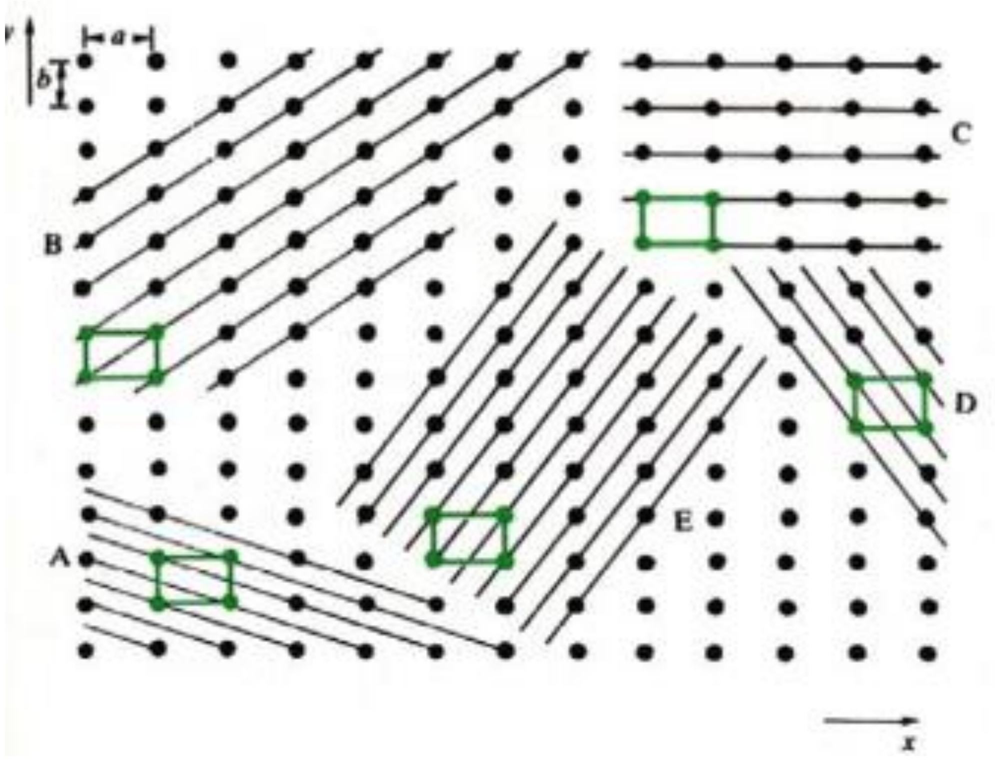
see, for instance,
Kittel chapter 2

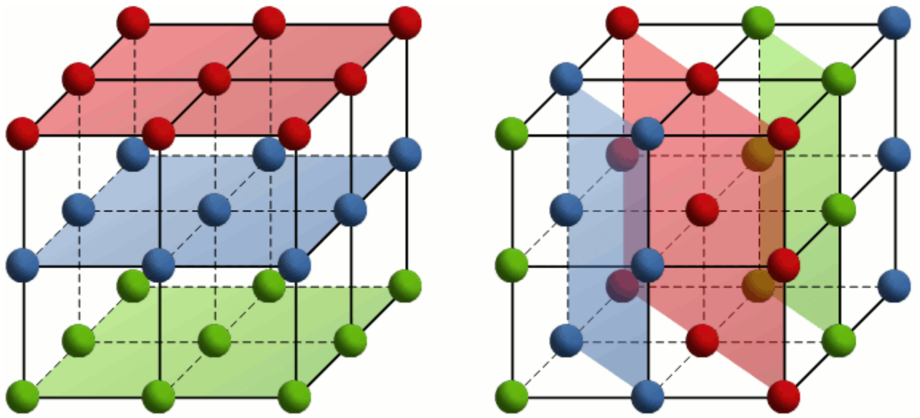
A crystal can also be seen as made up of equidistant planes



Lattice planes

A crystal lattice may be considered as an aggregate of a set of parallel equidistant planes of high density of lattices points



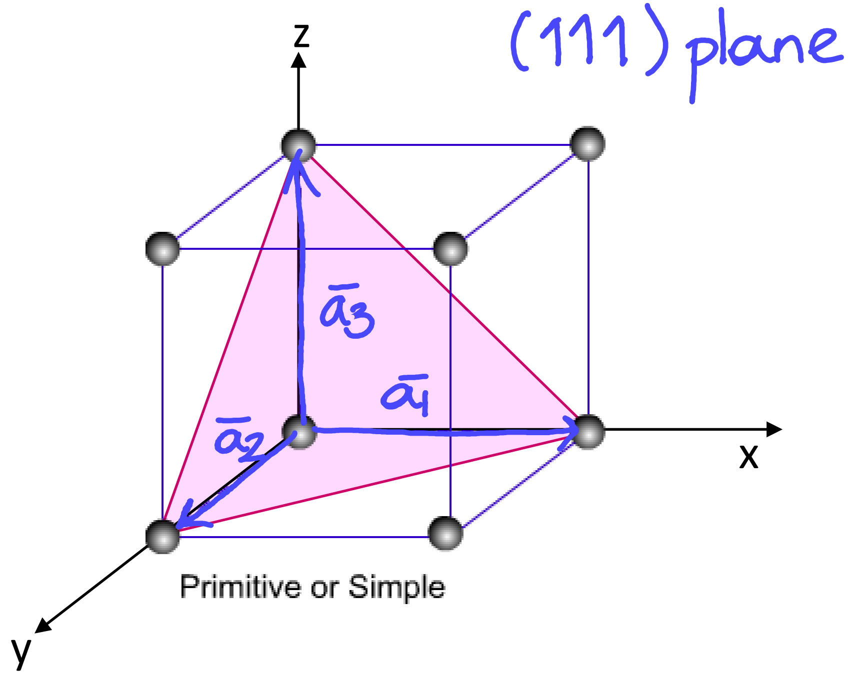


A ***lattice plane*** (or ***crystal plane***) is a plane containing at least three non-collinear (and therefore an infinite number of) points of the lattice

Lattice planes – Index system: Miller Indices

Miller indices are integers m_1, m_2 and m_3 that refer to the intercepts made by a plane on axes $\mathbf{a_1}$, $\mathbf{a_1}$ and $\mathbf{a_3}$.

- Determine the intercepts of the plane along the axes x, y and z in terms of the lattice constant a_1, a_2, a_3. $1a_1$ $1a_2$ $1a_3$
- Determine the reciprocals of these numbers: $1/m_1$, $1/m_2$, $1/m_3$. $1/1$ $1/1$ $1/1$
- Find the least common denominator (LCD) and multiply each by this lcd. (111)



The result is written in the form (hkl) and is called the Miller Indices of the plane.

Indices (hkl) might denote a single plane or a set of parallel planes

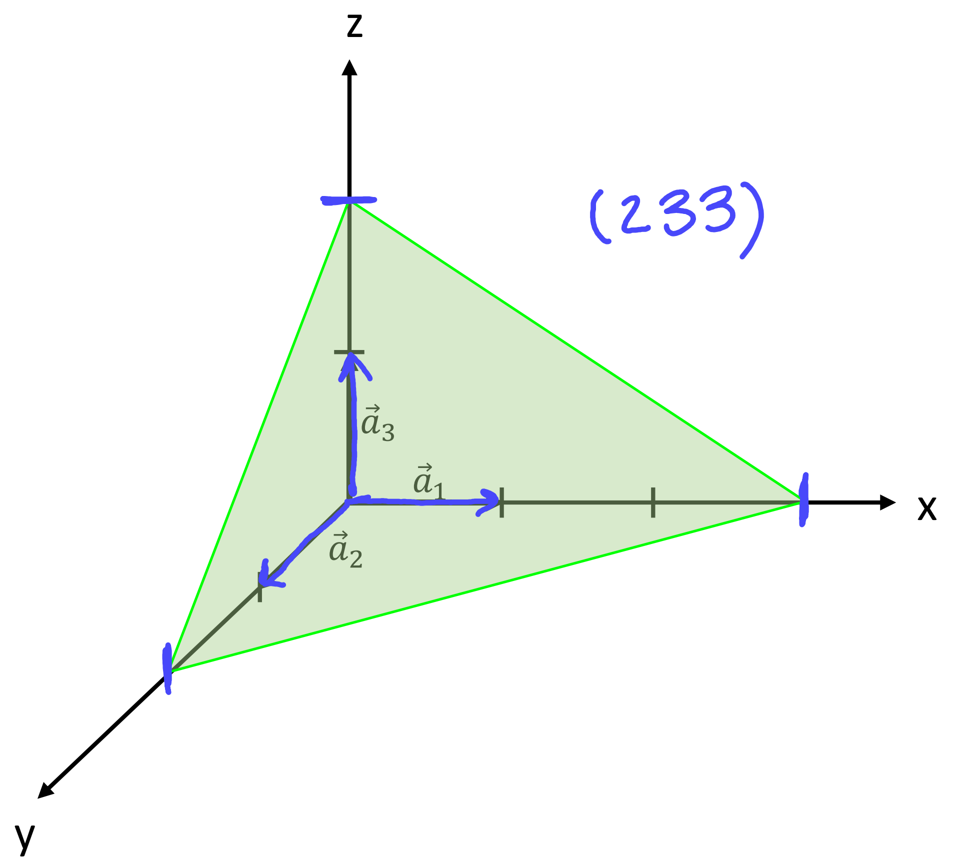
Lattice planes – Index system: Miller Indices

Miller indices are integers m_1, m_2 and m_3 that refer to the intercepts made by a plane on axes $\mathbf{a_1}$, $\mathbf{a_1}$ and $\mathbf{a_3}$.

- Determine the intercepts of the plane along the axes x, y and z in terms of the lattice constant a_1, a_2, a_3. $3a_1 \quad 2a_2 \quad 2a_3$
- Determine the reciprocals of these numbers: $1/m_1$, $1/m_2$, $1/m_3$. $1/3 \quad \frac{1}{2} \quad \frac{1}{2}$
- Find the least common denominator (LCD) and multiply each by this lcd. (233)

// Reduce them to integers having the same ratio (usually the smallest)

The result is written in the form (hkl) and is called the Miller Indices of the plane.

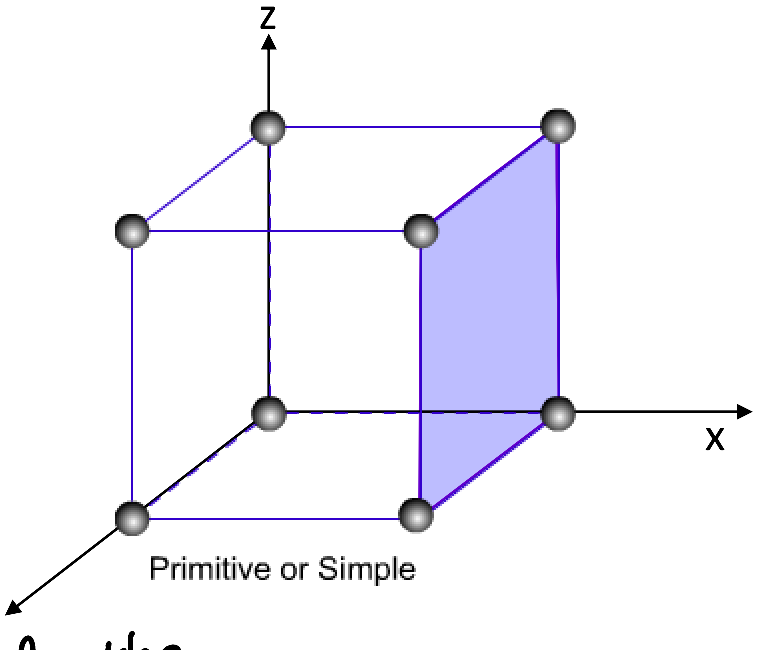


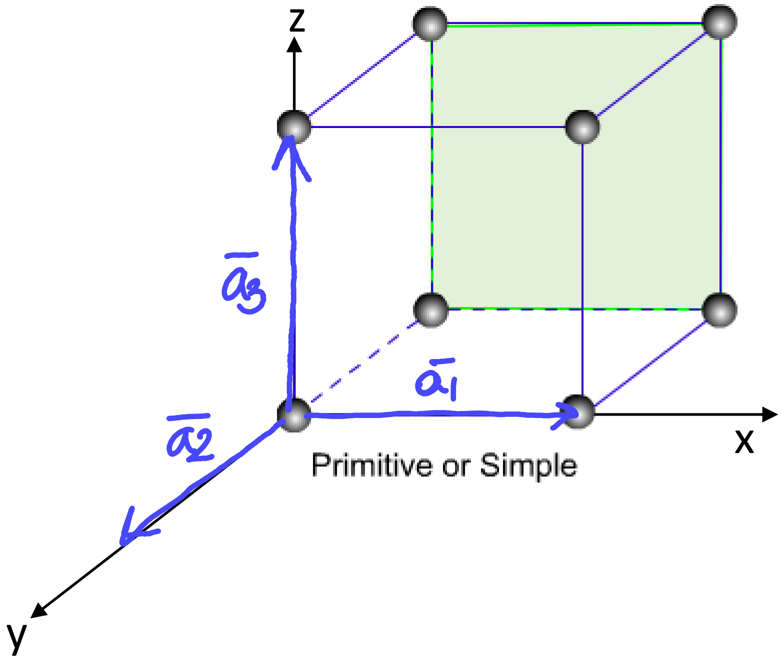
Lattice planes in cubic crystals

$\frac{1}{1}\ \frac{1}{0}\ \frac{1}{0} \longrightarrow (100)$

$(0\bar{1}0)$

it indicates that intercept at the negative side of the origin





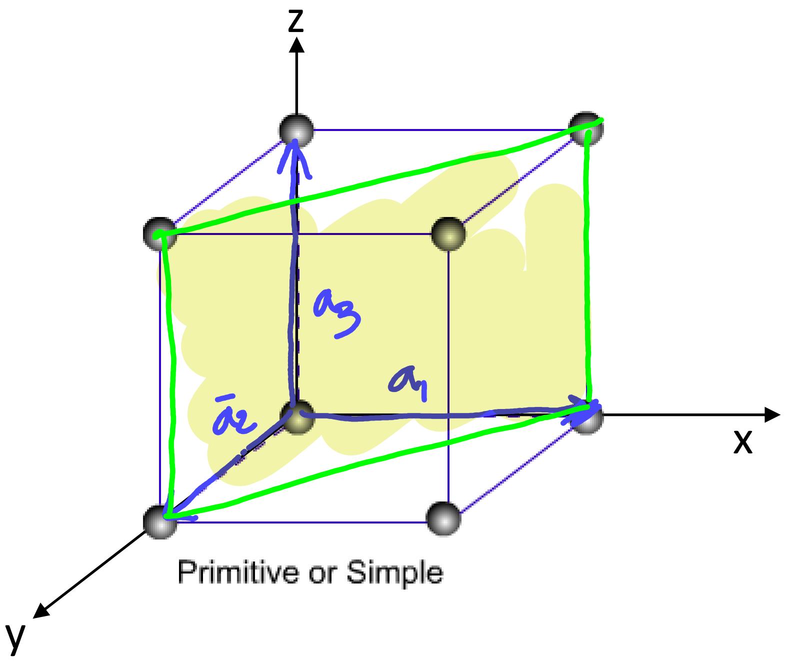
In a cubic crystal, the (001), (010), (100), $(00\bar{1})$, $(0\bar{1}0)$, $(\bar{1}00)$ planes are equivalent by symmetry

$\{100\}$

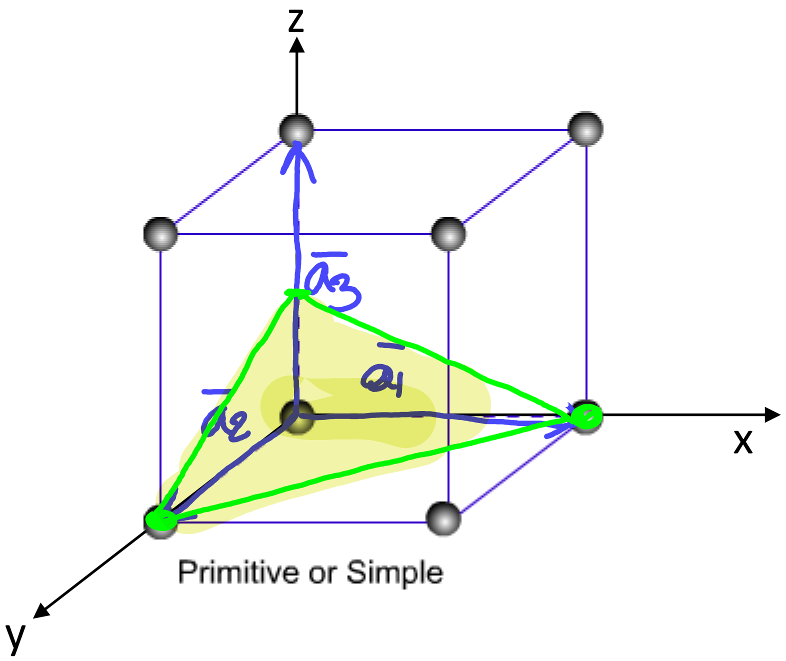
Draw a plane for the given Miller indices:

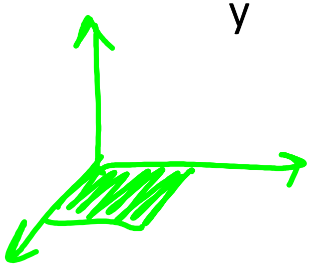
it cuts a_3 @ $\frac{1}{2}$

(110)

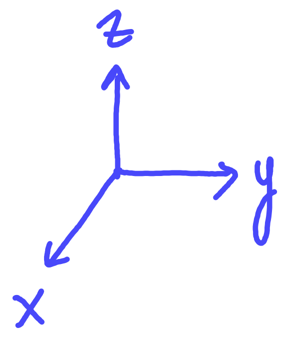


(112)

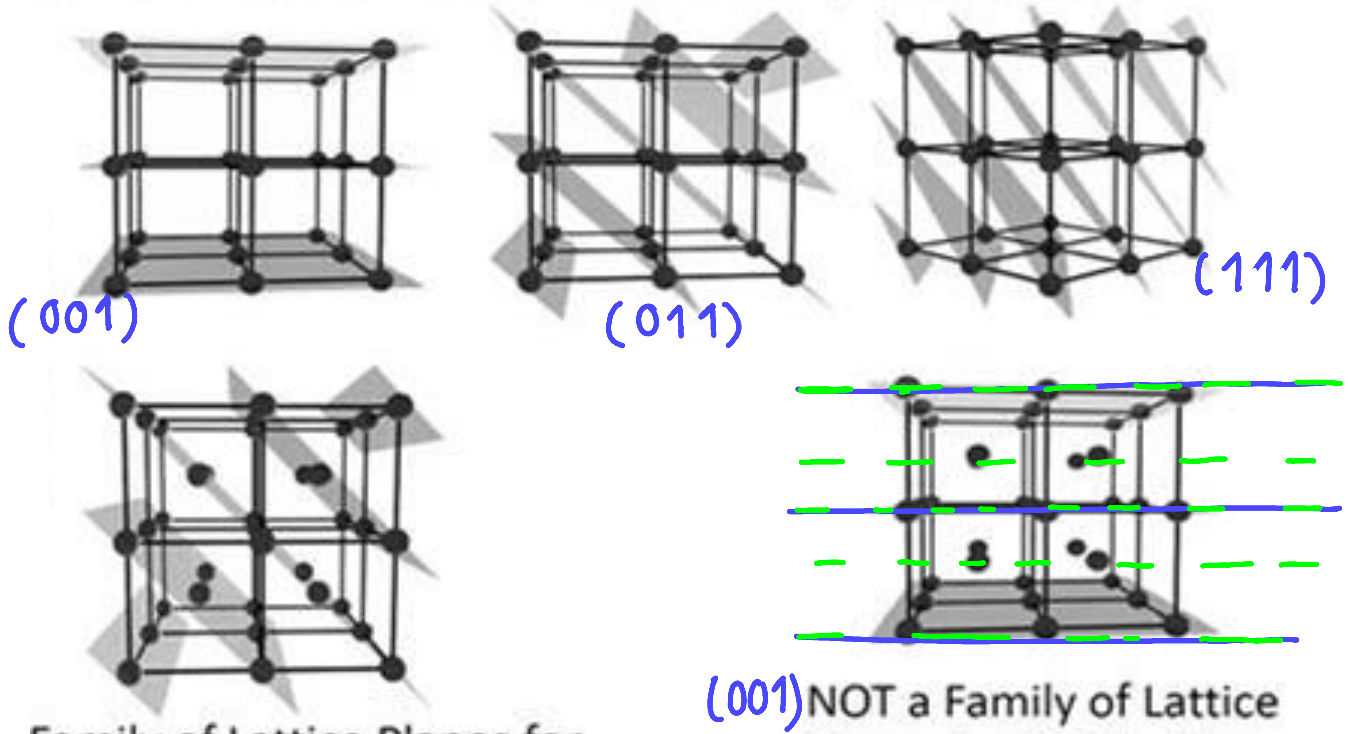




A ***family of lattice planes*** is an infinite set of equally separated parallel lattice planes which taken togther contain all points of the lattice



Some Families of Lattice Planes for Simple Cubic Lattice

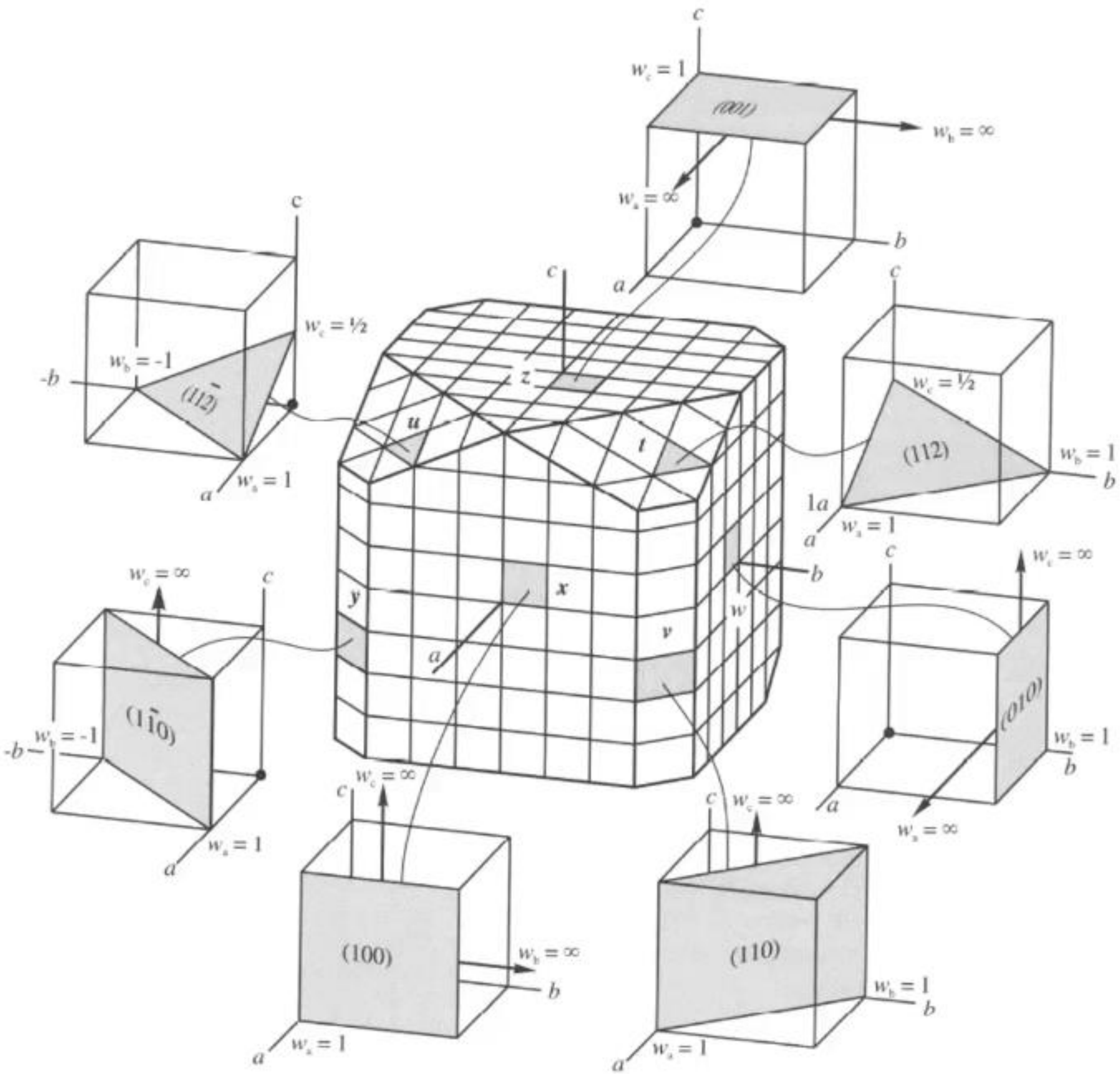


Family of Lattice Planes for BCC Lattice

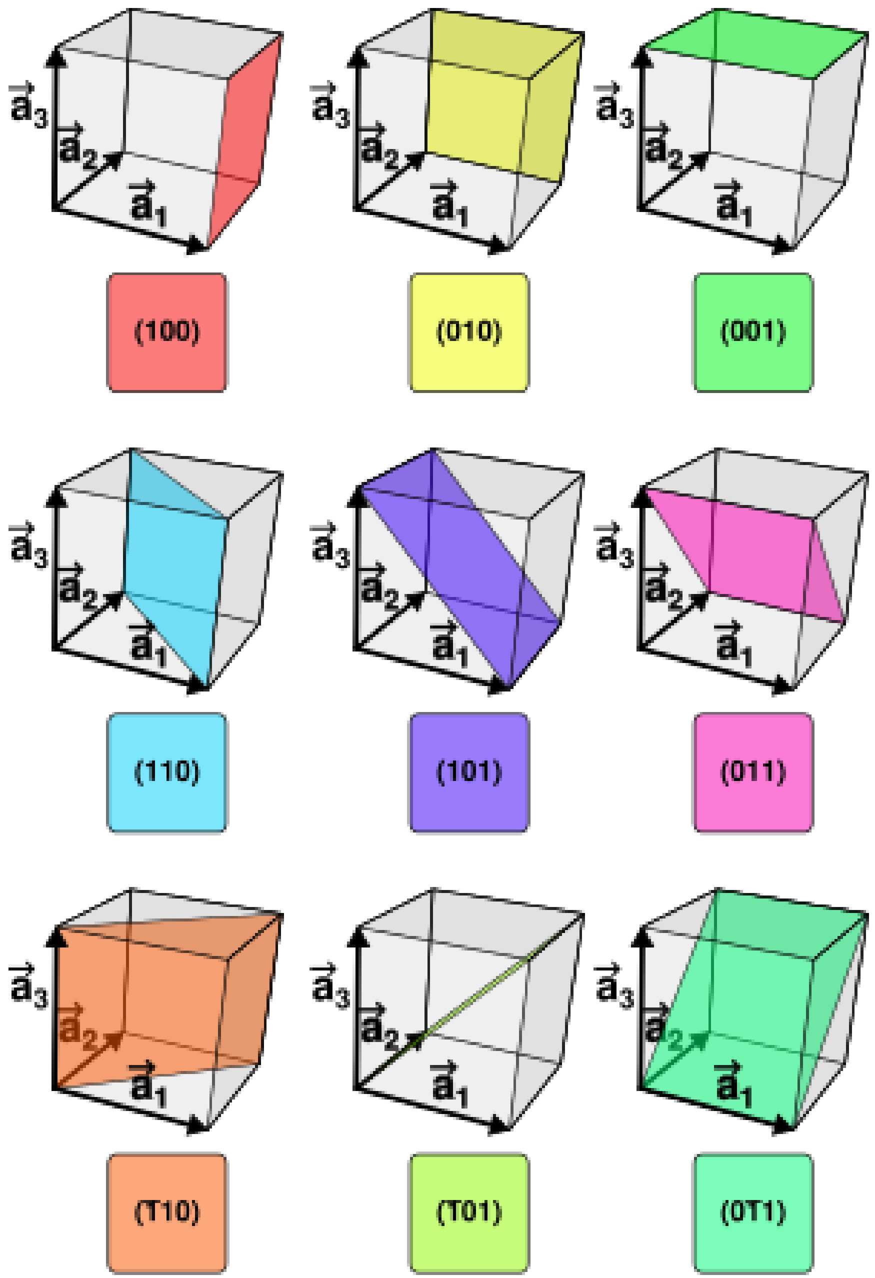
(001) NOT a Family of Lattice Planes for BCC Lattice

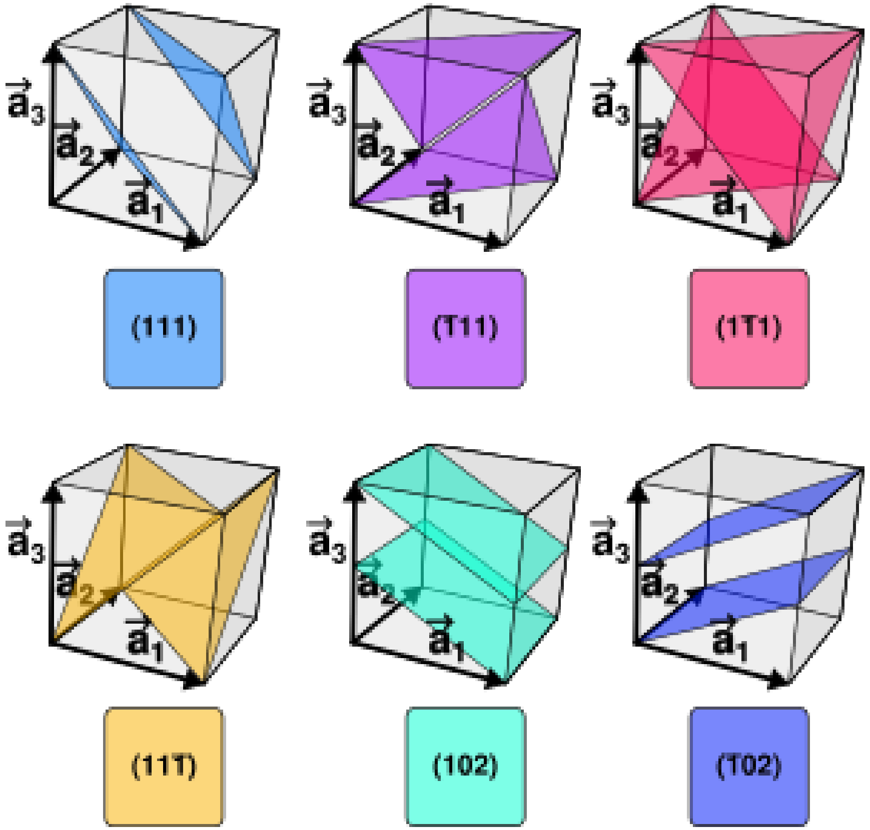
(002) is a valid family of lattice planes for the BCC

* plane (002): parallel to (001) but cutting a_3 at $\frac{1}{2}a$



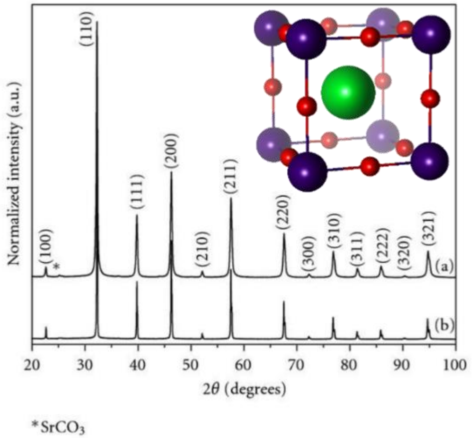
(001)
(112̄)
(112)
(11̄0)
(010)
(100)
(110)
$w_a = 1$
$w_b = -1$
$w_c = ½$
$w_a = \infty$
$w_b = \infty$
$w_c = 1$
$w_b = 1$
$w_c = \infty$
a
b
c
-b
u
t
z
x
y
v
w

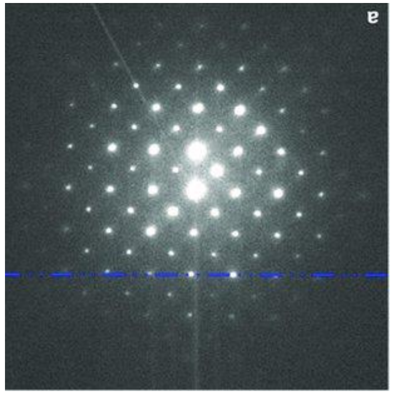

(100)
(010)
(001)
(110)
(101)
(011)
$(\bar{1}10)$
$(\bar{1}01)$
$(0\bar{1}1)$

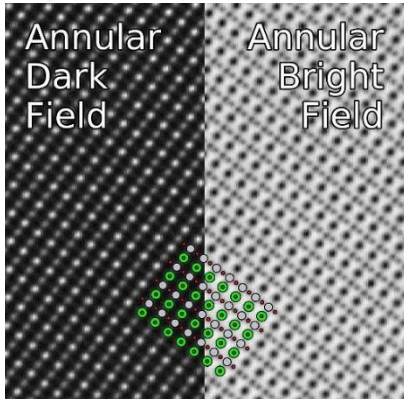

(111)
$(\bar{1}11)$
$(1\bar{1}1)$
$(11\bar{1})$
(102)
$(\bar{1}02)$

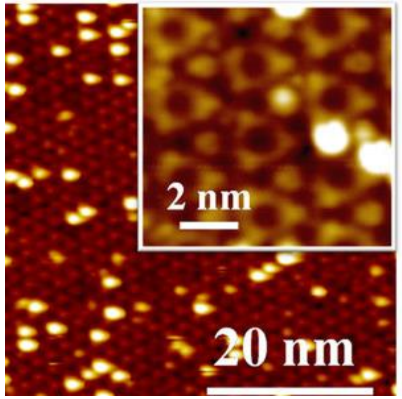
How can we study crystals?

A number of techniques allow to obtain experimental evidence of the periodicity of atomic structures:









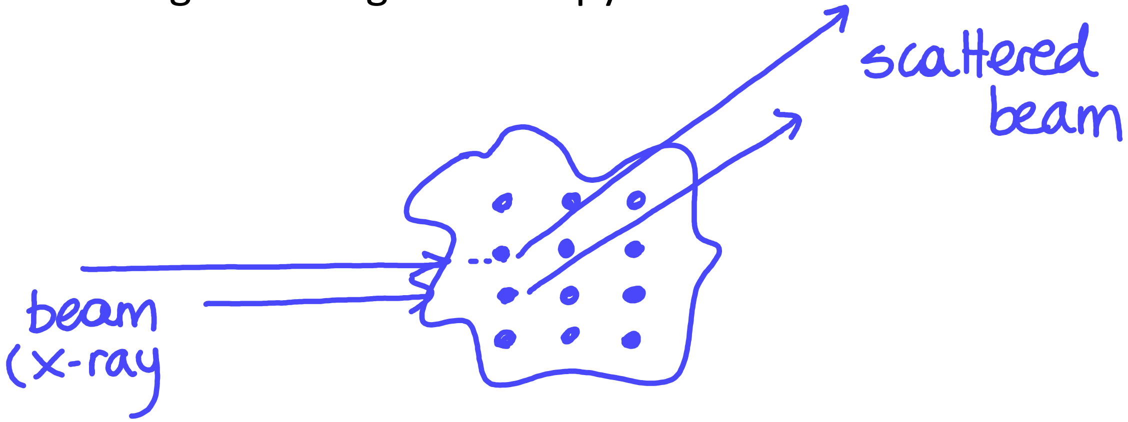
(1) x-ray diffraction

(2) neutron diffraction

(3) electron diffraction

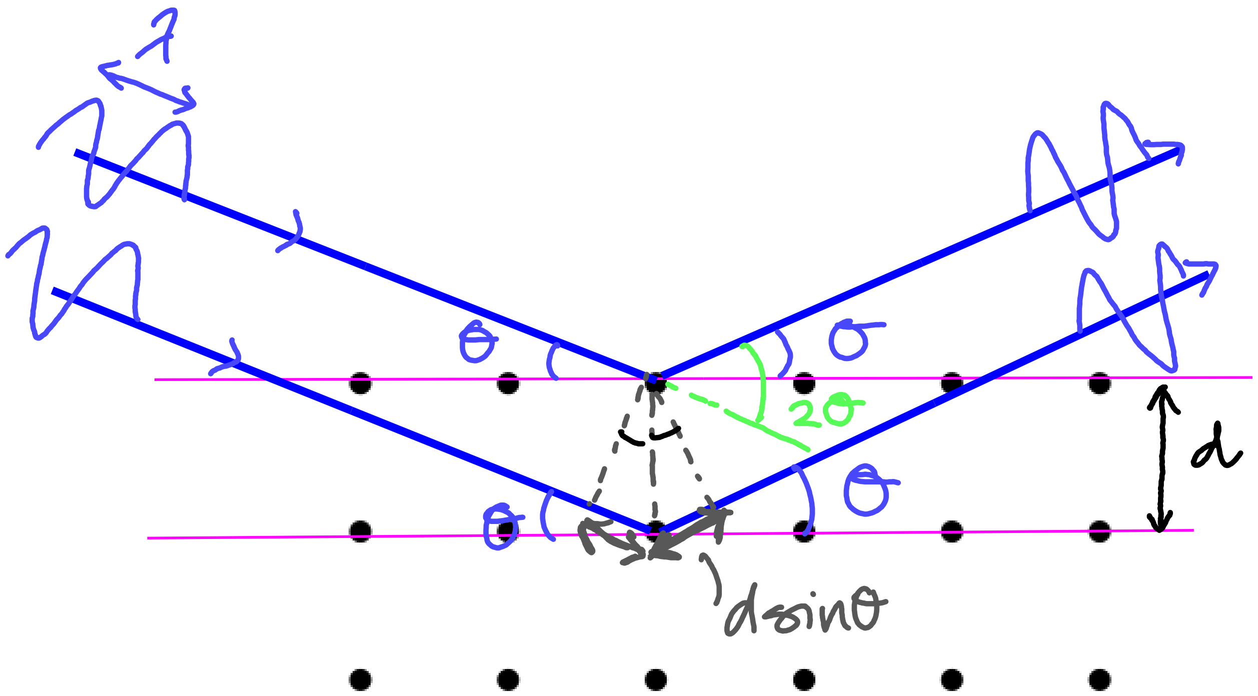
(4) High resolution electron microscopy

(5) Scanning tunneling microscopy



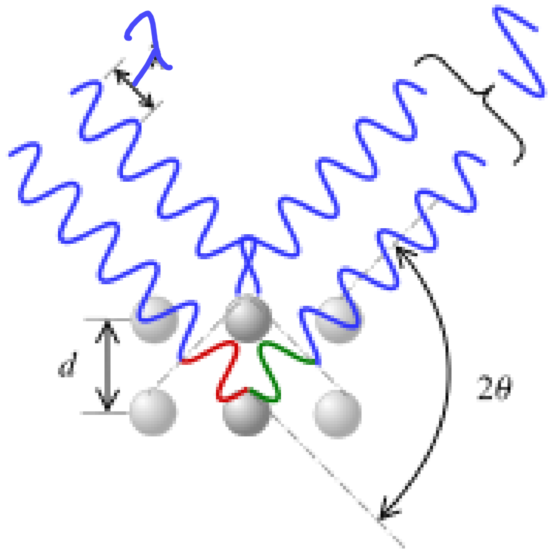
Diffraction: constructive interference of the scattering from a large number of cells.

Bragg Law

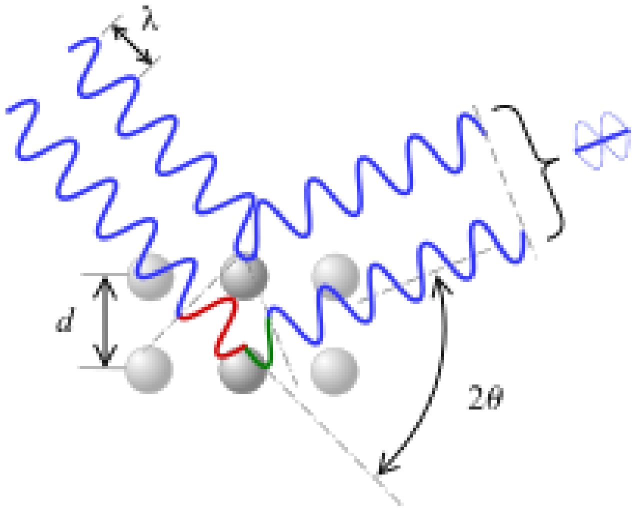


- Elastic scattering ($E = \hbar\omega$ is conserved)
- Condition for constructive interference : $\boxed{2d\sin\theta = n\lambda}$

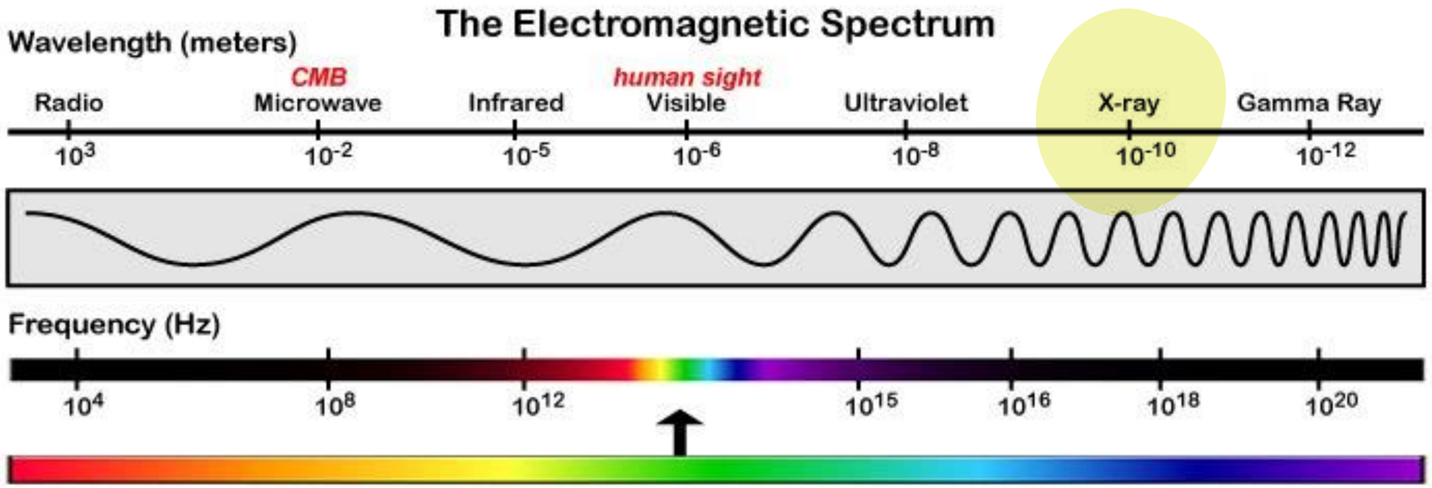
integer number

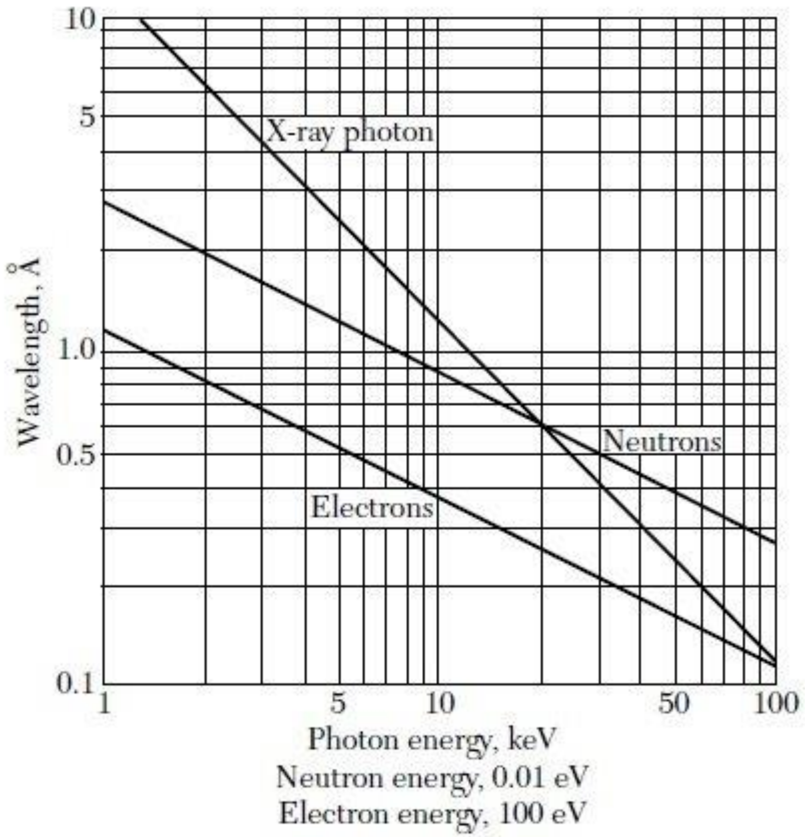


Constructive Interference



Destructive Interference



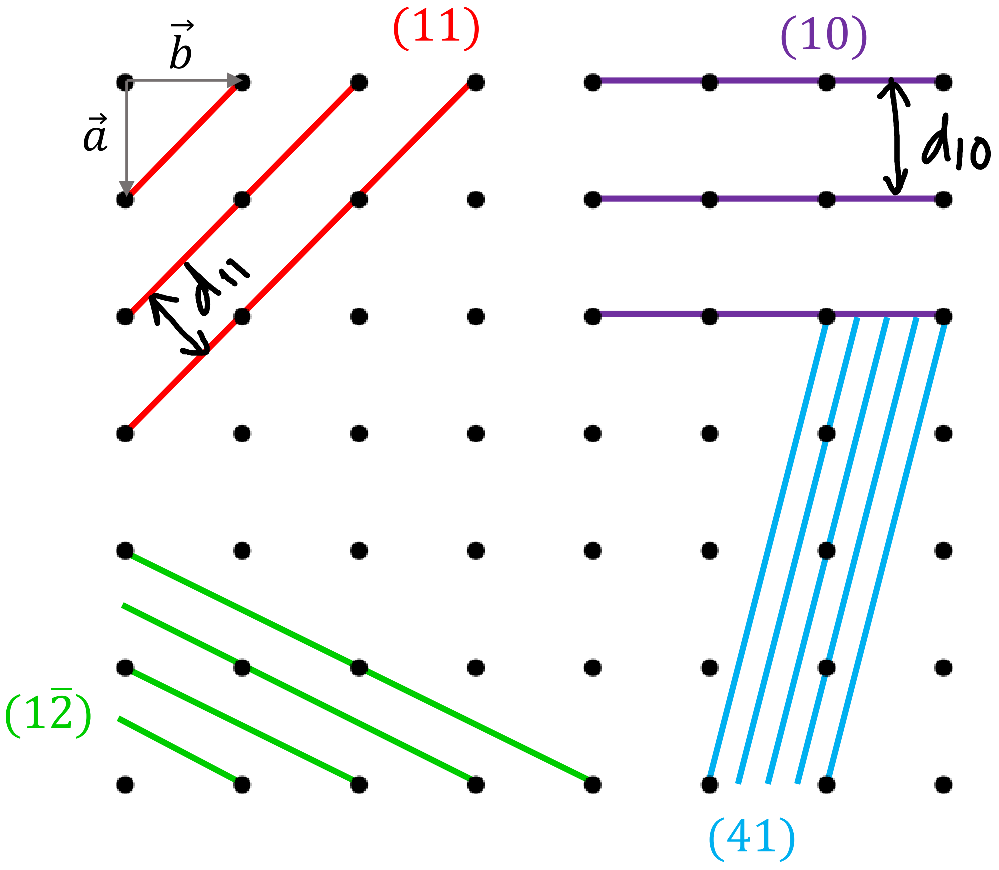


$$2d\sin\theta = n\lambda \implies \lambda \leq 2d$$

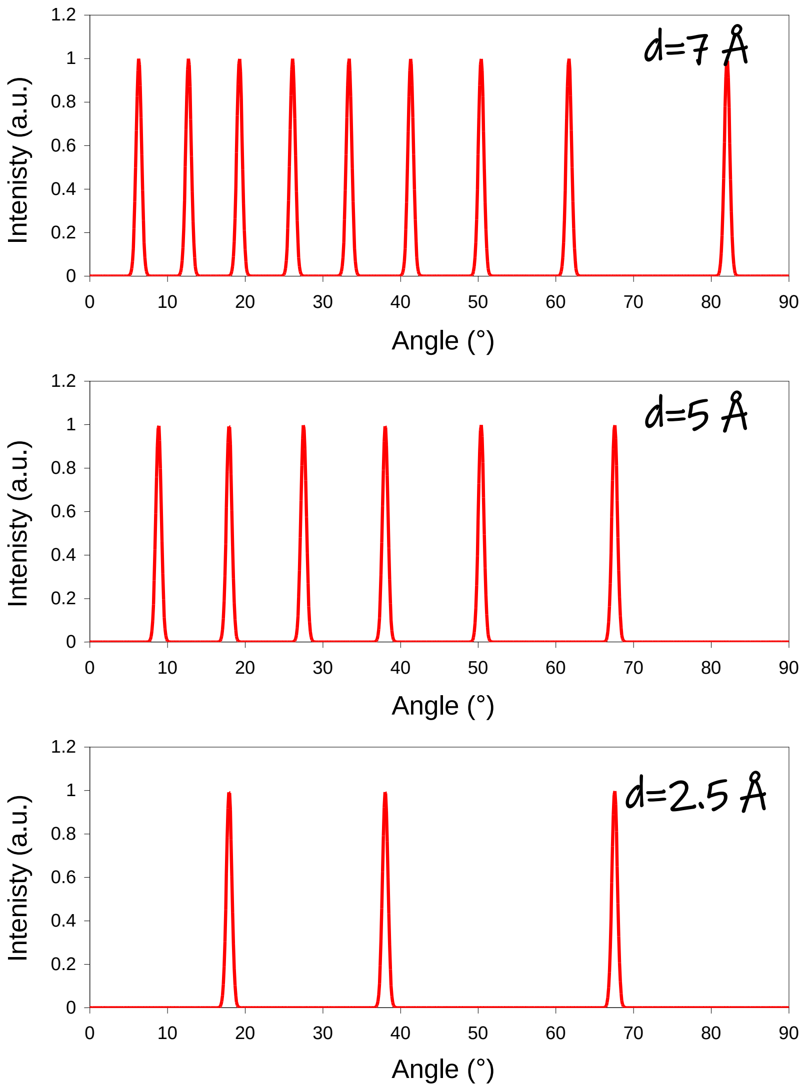
$$d \sim 5\,\text{Å}$$

Meaning of *d*

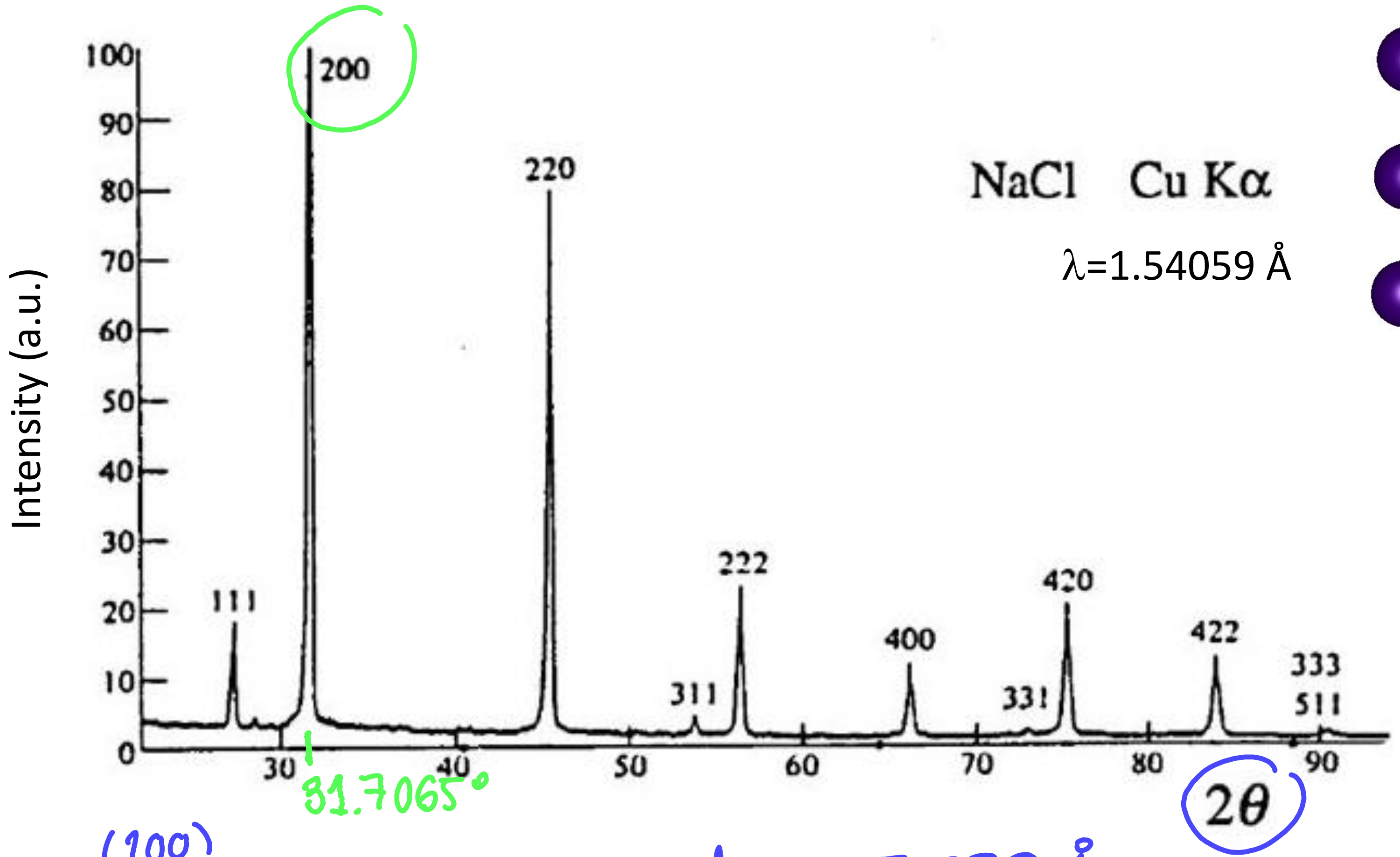
$$2d \sin\theta = n\lambda$$



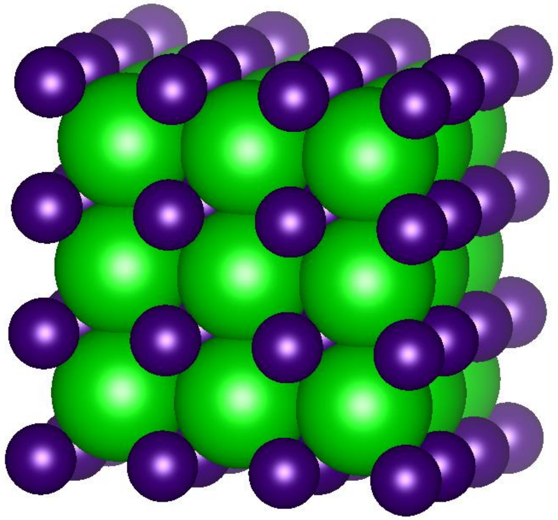
Simulated diffraction patterns for λ= 1.5406 Å
and different distance between planes



Determine the lattice parameter for NaCl



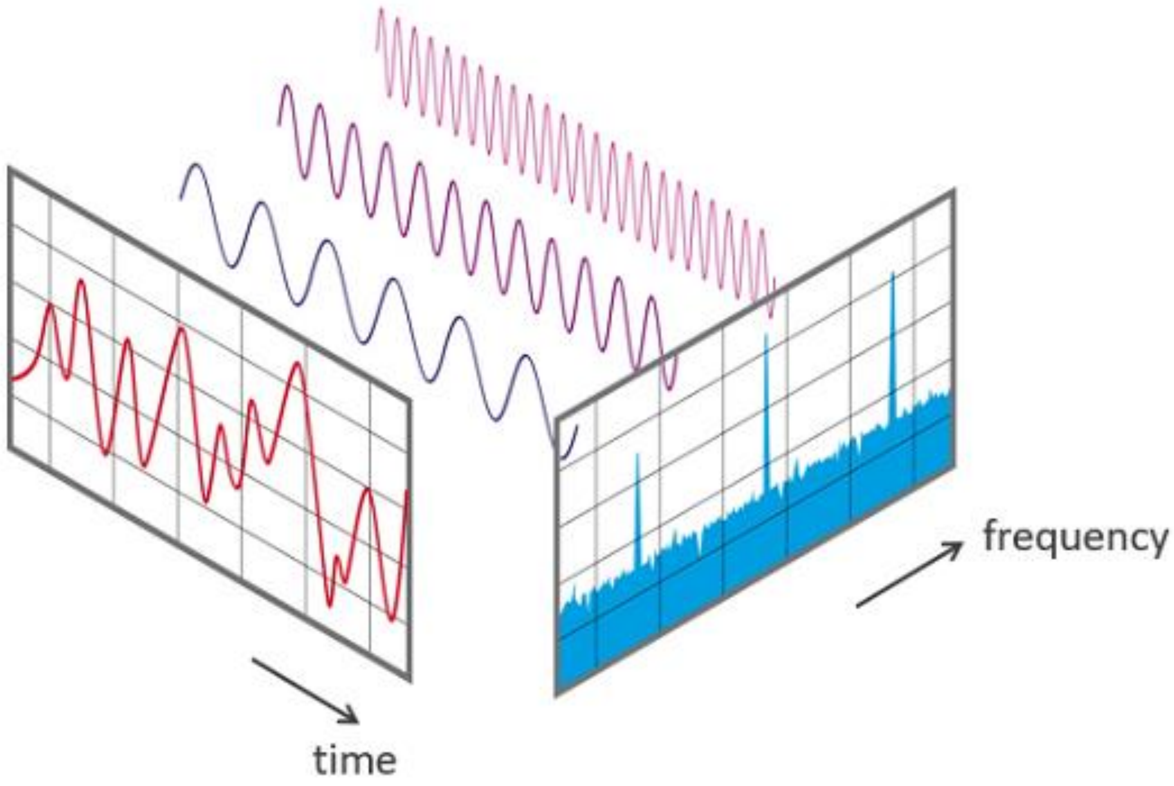
λ=1.54059 Å



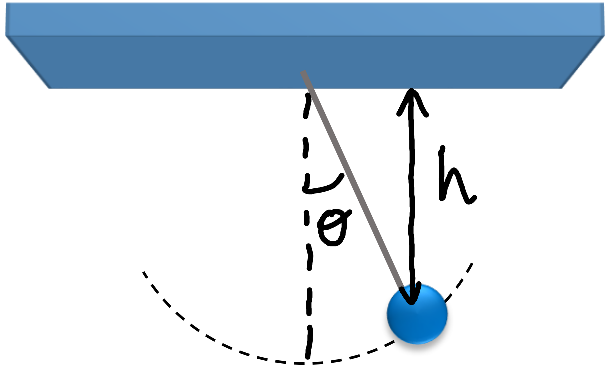
$2d\sin\theta = n\lambda$

$d = \frac{n\lambda}{2\sin\theta} \xrightarrow[n=2]{(200)}$ lattice parameter $= 5.639$ Å

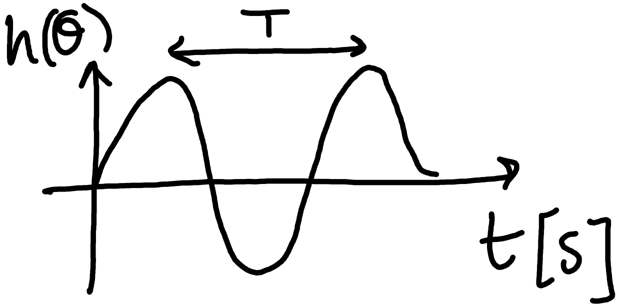
Fast Fourier transform



Analogy

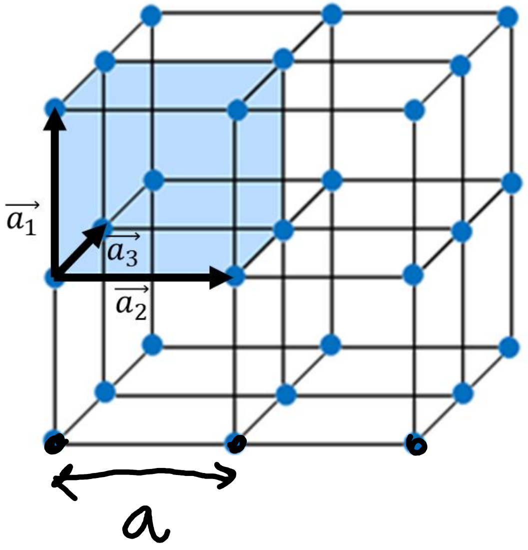


Real time



Reciprocal time

Angular freq: $\omega = \frac{2\pi}{T}$ $[s^{-1}]$



Real space

$$\vec{r}' = \vec{r} + \vec{T}$$

$$n(\vec{r}) = n(\vec{r} + \vec{T})$$

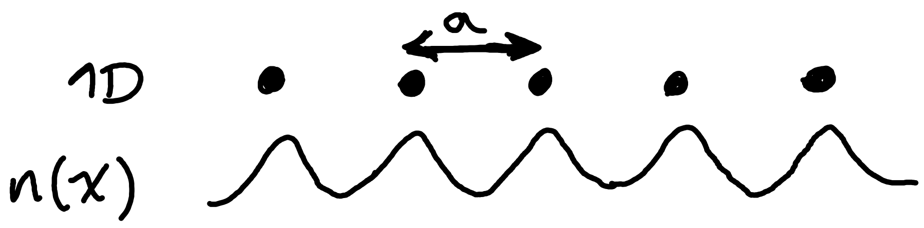
[Å]

Reciprocal space

$$\frac{2\pi}{a}$$

$[Å^{-1}]$

Fourier analysis



- crystal invariant under translation of the type $\vec{T} = u_1\bar{a}_1 + u_2\bar{a}_2 + u_3\bar{a}_3$
- Any physical property of the crystal will also be invariant under T
  Ex. electron density $n(\vec{r}+T) = n(\vec{r})$

Fourier analysis 1D

1D $\quad \vec{r} \to x \Rightarrow$ periodicity $n(x+a) = n(x)$

n: it can be expanded in a Fourier series

$$n(x) = n_0 + \sum_{p>0}\left[c_p \sin\left(\frac{2\pi}{a}px\right) + s_p \sin\left(\underbrace{\frac{2\pi}{a}}_{\text{to ensure periodicity}}px\right)\right]$$

p: positive integers $\quad$ Fourier coefficients $\quad$ to ensure periodicity

$$n(x+a) = n_0 + \sum_{p>0}\left[c_p \cos\left(\frac{2\pi}{a}px + \frac{2\pi}{\cancel{a}}p\cancel{a}\right) + s_p \sin\left(\frac{2\pi}{a}px + \frac{2\pi}{\cancel{a}}p\cancel{a}\right)\right] = n(x) \checkmark$$

Fourier analysis (1D)

Complex notation is useful because it is more compact:

$$n(x) = \sum_{p \in \mathbb{Z}} n_p \exp\left(i \frac{2\pi}{a} x\right) \qquad n(x+a) = n(x)$$

all integers

complex number: to ensure $n(x)$ is real: $n_{-p}^* = n_p$

$$G_p \equiv \frac{2\pi}{a} p = 0, \pm \frac{2\pi}{a}, \pm \frac{4\pi}{a} \ldots$$

these points constitute the reciprocal lattice in Fourier space

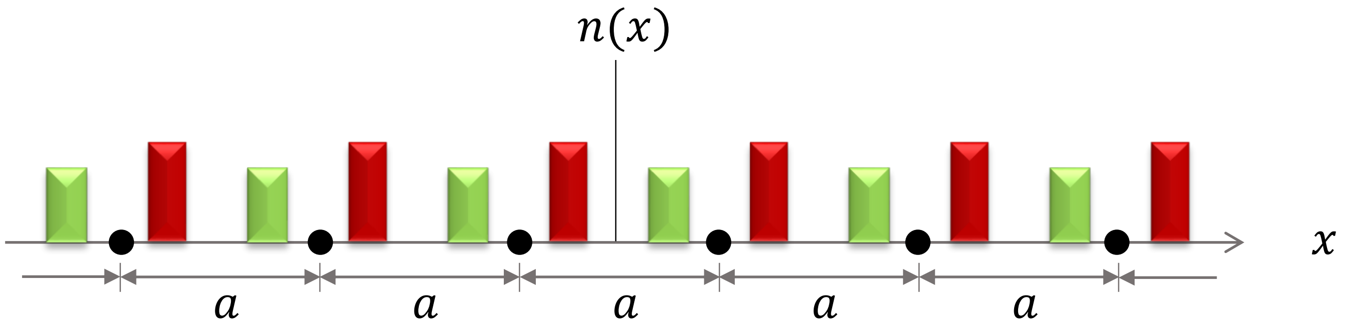
We can also write the periodic function: $\boxed{n(x) = \sum_p n_p e^{i G_p x}}$

analogy: each G_p would be the harmonic and n_p its amplitude https://www.falstad.com/fourier/

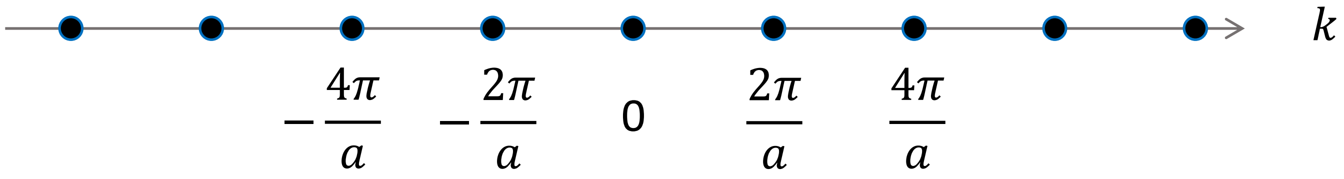
Real and reciprocal lattice in 1D

Real Lattice

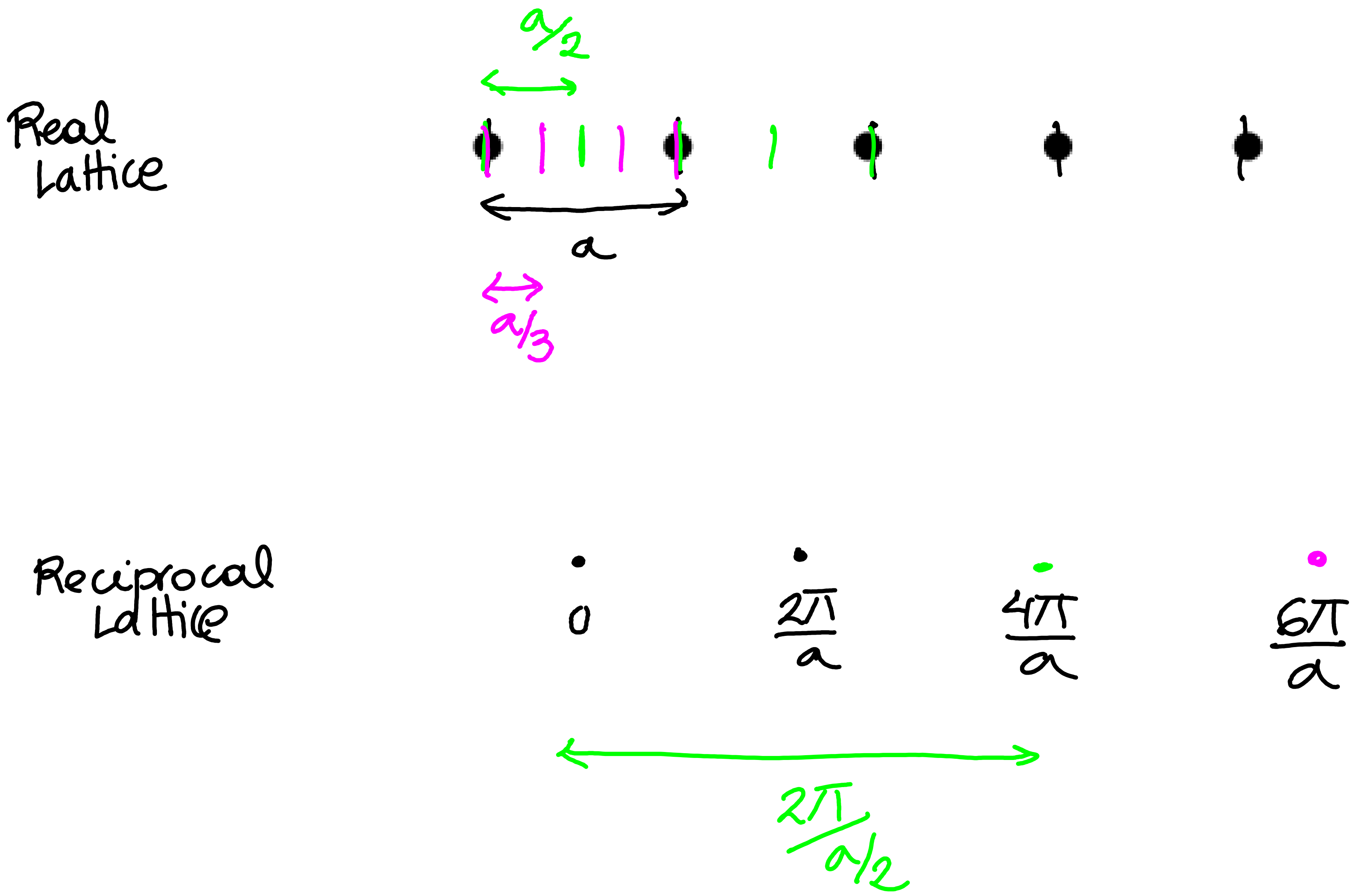
periodic function $n(x)$ of period a



Reciprocal Lattice



How is the Reciprocal Lattice conctructed



Reciprocal Lattice vectors

in 1D $G_p = \frac{2\pi}{a} p$

3D $$\boxed{n(\vec{r}) = \sum_{\vec{G}} n_{\vec{G}} \exp(i\vec{G}\cdot\vec{r})}$$

If $\vec{a}_1$, $\vec{a}_2$ and $\vec{a}_3$are primitive vectors of the crystal lattice, the reciprocal lattice can be generated by:

$$\vec{b}_1 = 2\pi \frac{\vec{a}_2 \times \vec{a}_3}{\vec{a}_1 \cdot \vec{a}_2 \times \vec{a}_3}$$

$$\vec{b}_2 = 2\pi \frac{\vec{a}_3 \times \vec{a}_1}{\vec{a}_1 \cdot \vec{a}_2 \times \vec{a}_3}$$

$$\vec{b}_3 = 2\pi \frac{\vec{a}_1 \times \vec{a}_2}{\vec{a}_1 \cdot \vec{a}_2 \times \vec{a}_3} \rightarrow \frac{2\pi}{V_c} \bar{a}_1 \times \bar{a}_2$$

$$\vec{b}_i \cdot \vec{a}_i = 2\pi \delta_{ij}$$

$\delta_{ij} = 1 \quad i = j$

$\delta_{ij} = 0 \quad i \neq j$

$\bar{b}_2 \cdot \bar{a}_2 = 2\pi$

$\bar{b}_2 \cdot \bar{a}_1 = 0$

$\bar{a}_1, \bar{a}_2, \bar{a}_3$ are primitive Lattice vectors

$\bar{b}_1, \bar{b}_2, \bar{b}_3$ will be primitive vectors of the reciprocal Lattice

Reciprocal Lattice

any point of the reciprocal lattice can be described by the reciprocal lattice vector $\vec{G} = h\bar{b}_1 + K\bar{b}_2 + \ell\bar{b}_3$ with $h, K, \ell = 0, \pm 1, \pm 2 \ldots$

these $\bar{G}$ vectors are the ones entering the Fourier series

$$n(\vec{r}) = \sum_{G} n_G \exp(i\bar{G}\vec{r})$$

$$T = u_1\bar{a}_1 + u_2\bar{a}_2 + u_3\bar{a}_3$$

given that the crystal is invariant under $\vec{T}$:

$$n(\vec{r}+\vec{T}) = \sum_{G} n_G \exp(i\vec{G}(\vec{r}+\vec{T})) = \sum_{G} n_G \exp(i\bar{G}\bar{r})\underbrace{\exp(i\bar{G}\bar{T})}_{=1} = n(\vec{r}) \checkmark$$

$$\vec{G}.\vec{T} = 2\pi\underbrace{(hu_1 + Ku_2 + \ell u_3)}_{} = 2\pi p \rightarrow \exp(iGT) = 1$$

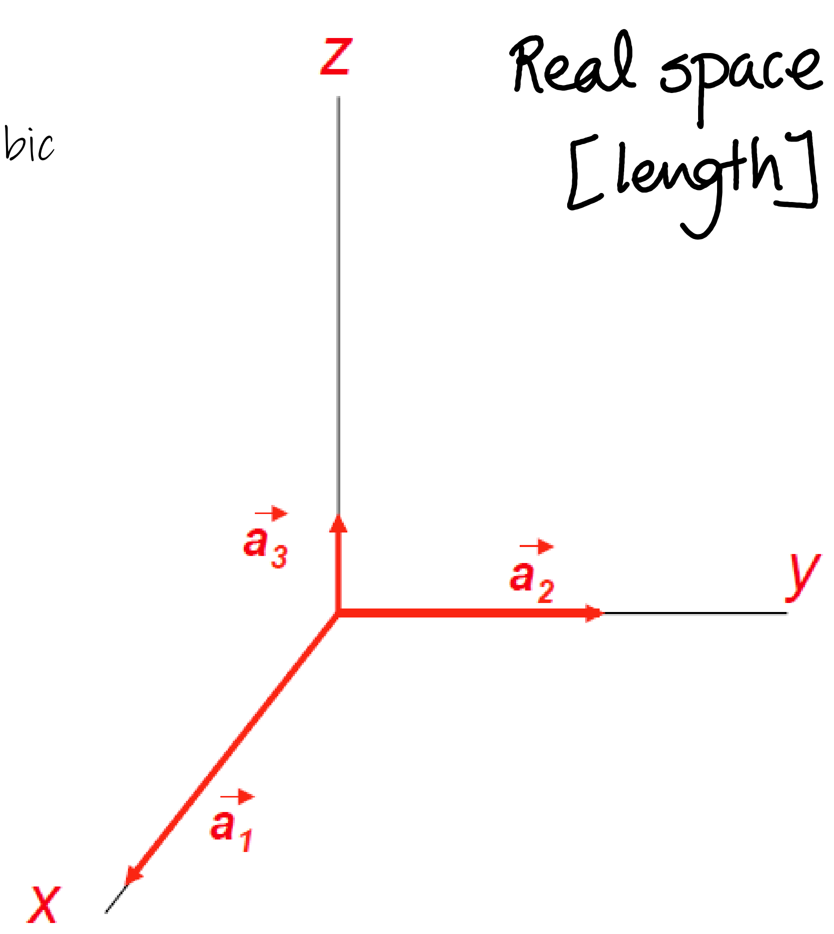
$b_i . a_j = 2\pi\delta_{ij}$

$$\boxed{e^{i\vec{G}.\vec{T}} = 1}$$

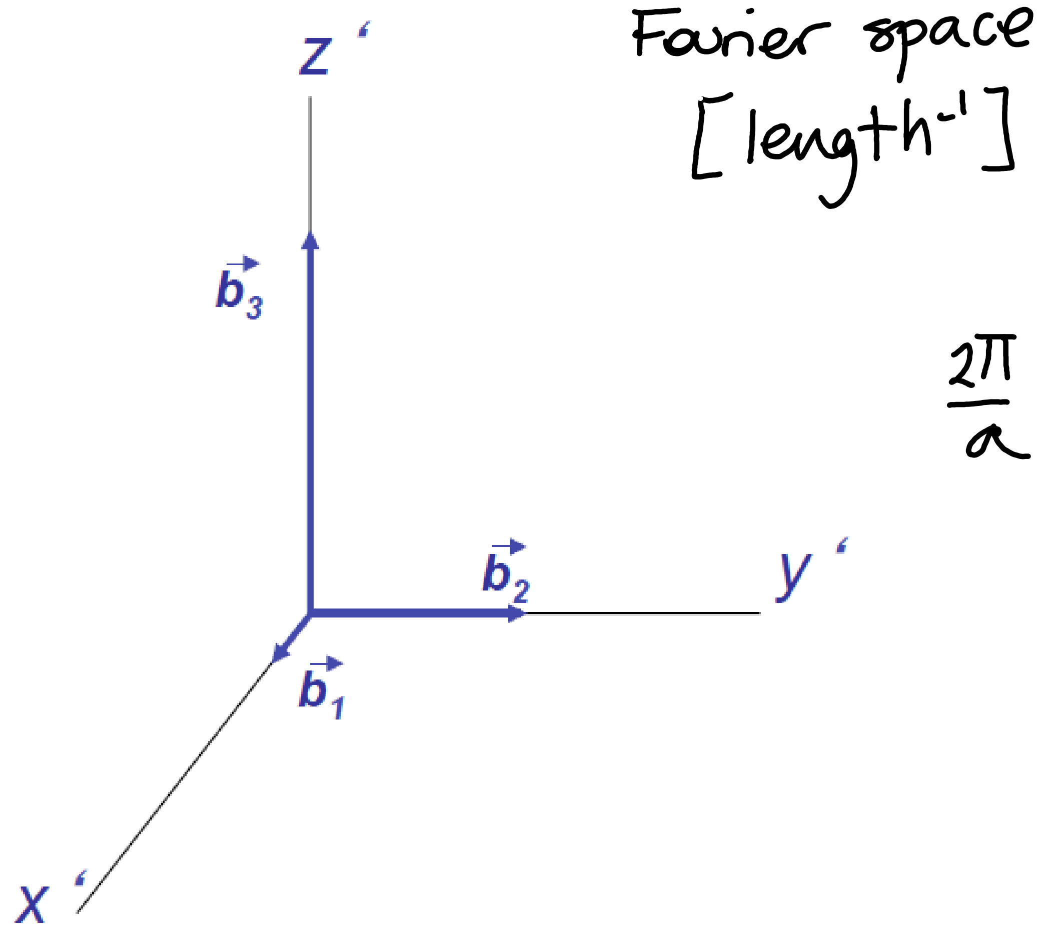
Vectors of the reciprocal lattice are defined through this expression

So, every crystal has 2 lattice associated:

Orthorhombic cell



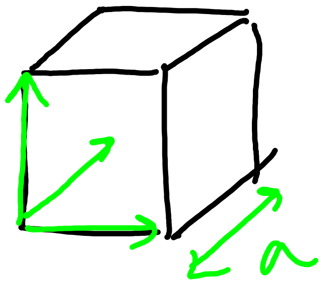
Crystal lattice



Reciprocal lattice

Reciprocal lattices in 3D

Reciprocal lattice to simple cubic



$\vec{a}_1 = a\hat{x}$ $\quad\quad$ $\vec{a}_2 = a\hat{y}$ $\quad\quad$ $\vec{a}_3 = a\hat{z}$

$$\vec{b}_1 = 2\pi \frac{\vec{a}_2 \times \vec{a}_3}{\vec{a}_1 \cdot \vec{a}_2 \times \vec{a}_3}$$

$$\vec{b}_2 = 2\pi \frac{\vec{a}_3 \times \vec{a}_1}{\vec{a}_1 \cdot \vec{a}_2 \times \vec{a}_3}$$

$$\vec{b}_3 = 2\pi \frac{\vec{a}_1 \times \vec{a}_2}{\vec{a}_1 \cdot \vec{a}_2 \times \vec{a}_3}$$

$\vec{b}_1 = \frac{2\pi}{a}\hat{x}$ $\quad\quad$ $\vec{b}_2 = \frac{2\pi}{a}\hat{y}$ $\quad\quad$ $\vec{b}_3 = \frac{2\pi}{a}\hat{z}$

the reciprocal lattice of a simple cube is a cube of lattice constant $\frac{2\pi}{a}$

A ***lattice plane*** (or ***crystal plane***) is a plane containing at least three non-collinear (and therefore an infinite number of) points of the lattice

A ***family of lattice planes*** is an infinite set of equally separated parallel lattice planes which taken together contain all points of the lattice

Reciprocal lattice points as families of lattice planes

The families of lattice planes there are in one-to-one correspondence with the possible directions of the reciprocal lattice vectors, to which they are normal.

For a family of planes separated d,

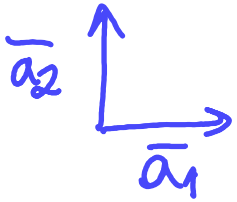
The reciprocal vector $\vec{G} = h\vec{b}_1 + k\vec{b}_2 + l\vec{b}_3$ is perpendicular to the real lattice plane with index hkl.

Further, the spacing between these lattice planes is

$$d = \frac{2\pi}{\left|\vec{G}_{min}\right|}$$

where $\vec{G}_{min}$ is the minimum length reciprocal lattice vector in this normal direction.

Square Lattice

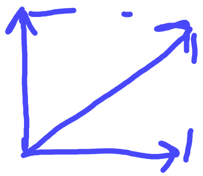


$$\bar T = u_1\bar a_1 + u_2\bar a_2$$

$$\left.\begin{aligned}\bar a_1 &= a\,(1,0)\\ \bar a_2 &= a\,(0,1)\end{aligned}\right\}\qquad \begin{aligned}\bar b_1 &= \frac{2\pi}{a}\,(1,0)\\ \bar b_2 &= \frac{2\pi}{a}\,(0,1)\end{aligned}$$

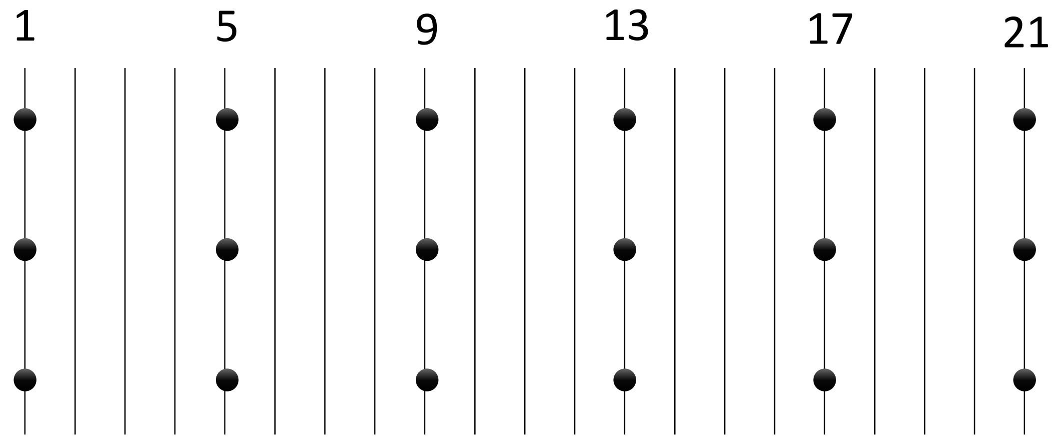
Ex. 1) $\vec G_1 = \bar b_1$ $\qquad d_{10} = \dfrac{2\pi}{|G|} = \dfrac{2\pi}{2\pi/a} = a$

Ex 2) $\vec G_2 = \bar b_1 + \bar b_2$ $\qquad d_{11} = \dfrac{2\pi}{|G|} = \dfrac{2\pi}{\frac{2\pi}{a}\sqrt{2}} = \dfrac{a}{\sqrt{2}} = \dfrac{a\sqrt{2}}{2}$



$$\vec G = h\bar b_1 + k b_2$$

Quiz



- Determine the reciprocal lattice vectors associated to

  a) 1, 9, 17, …
  b) 1, 5, 9, …
  c) 1, 3, 5, …
  d) 1, 2, 3, 4, …
  e) 1, 2, 5, 6, ….