Handout 5

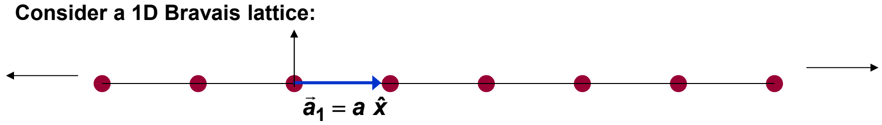
The Reciprocal Lattice

In this lecture you will learn:

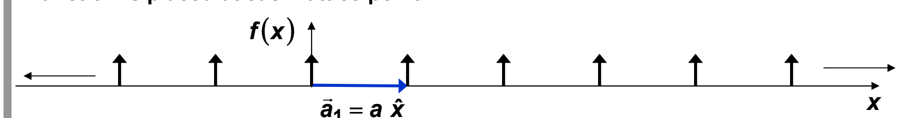
- Fourier transforms of lattices
- The reciprocal lattice
- Brillouin Zones
- X-ray diffraction
- Fourier transforms of lattice periodic functions

Fourier Transform (FT) of a 1D Lattice

Consider a 1D Bravais lattice:



Now consider a function consisting of a "lattice" of delta functions – in which a delta function is placed at each lattice point:



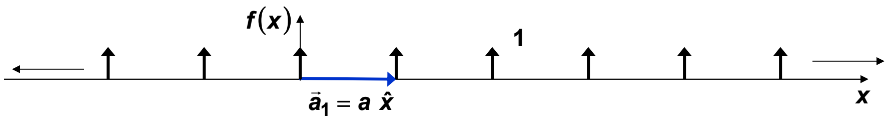
$$f(x) = \sum_{n=-\infty}^{\infty} \delta(x - n\,a)$$

The FT of this function is (as you found in your homework):

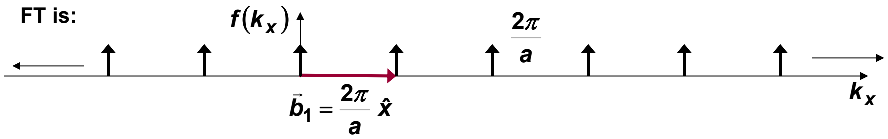
$$f(k_x) = \int_{-\infty}^{+\infty} dx \sum_{n=-\infty}^{\infty} \delta(x - n\,a)\, e^{-i\,k_x\,x} = \sum_{n=-\infty}^{\infty} e^{i\,k_x\,n\,a} = \frac{2\pi}{a} \sum_{m=-\infty}^{\infty} \delta\!\left(k_x - m\,\frac{2\pi}{a}\right)$$

The FT of a train of delta functions is also a train of delta functions in k-space

Reciprocal Lattice as FT of a 1D Lattice

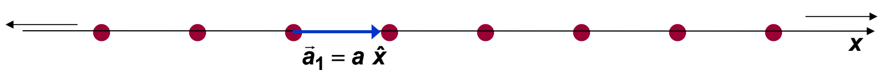


FT is:

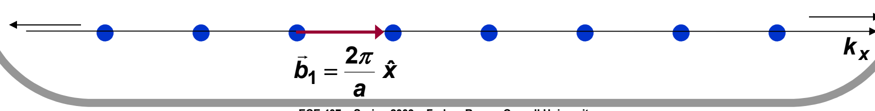


The reciprocal lattice is defined by the position of the delta-functions in the FT of the actual lattice (also called the direct lattice)

Direct lattice (or the actual lattice):

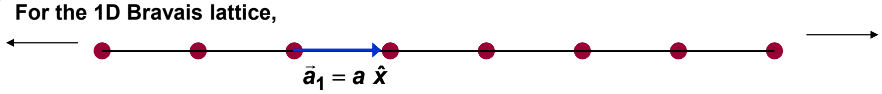


Reciprocal lattice:

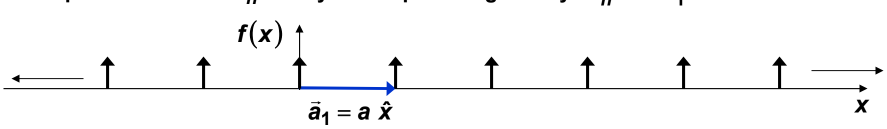


Reciprocal Lattice of a 1D Lattice

For the 1D Bravais lattice,



The position vector $\vec{R}_n$ of any lattice point is given by: $\vec{R}_n = n\,\vec{a}_1$



$$f(x) = \sum_{n=-\infty}^{\infty} \delta\left(\vec{x} - \vec{R}_n\right)$$

The FT of this function is: $f(k_x) = \int_{-\infty}^{+\infty} dx \sum_{n=-\infty}^{\infty} \delta\left(\vec{x} - \vec{R}_n\right) e^{-i\,k_x\,x} = \sum_{n=-\infty}^{\infty} e^{i\,\vec{k}.\vec{R}_n}$

The reciprocal lattice in k-space is defined by the set of all points for which the k-vector satisfies,

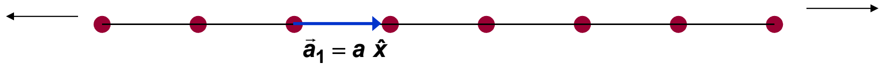
$$e^{i\,\vec{k}\,.\,\vec{R}_n} = 1$$

for ALL $\vec{R}_n$ of the direct lattice

For the points in k-space belonging to the reciprocal lattice the summation $\sum_{n=-\infty}^{\infty} e^{i\,\vec{k}.\vec{R}_n}$ becomes very large!

Reciprocal Lattice of a 1D Lattice

For the 1D Bravais lattice,



The position vector $\vec{R}_n$ of any lattice point is given by: $\vec{R}_n = n\,\vec{a}_1$

> The reciprocal lattice in k-space is defined by the set of all points for which the k-vector satisfies,
> $$e^{i\,\vec{k}\,.\,\vec{R}_n} = 1$$
> for ALL $\vec{R}_n$ of the direct lattice

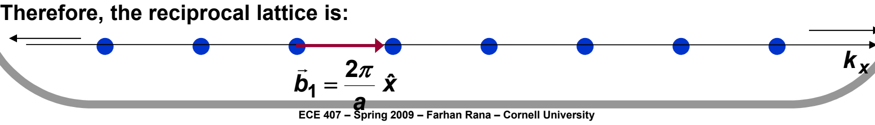
For $\vec{k}$ to satisfy $e^{i\,\vec{k}\,.\,\vec{R}_n} = 1$, it must be that for all $\vec{R}_n$:

$$\vec{k}\,.\,\vec{R}_n = 2\pi \times \{\text{integer}\}$$

$$\Rightarrow k_x\, na = 2\pi \times \{\text{integer}\}$$

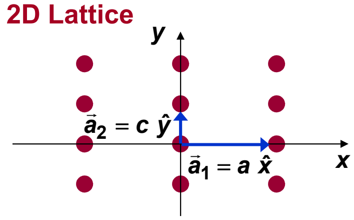
$$\Rightarrow k_x = m\frac{2\pi}{a} \quad \Big\{ \text{ where } m \text{ is any integer}$$

Therefore, the reciprocal lattice is:



Reciprocal Lattice of a 2D Lattice

Consider the 2D rectangular Bravais lattice:



If we place a 2D delta function at each lattice point we get the function:

$$f(x,y) = \sum_{n=-\infty}^{\infty}\sum_{m=-\infty}^{\infty} \delta(x - n\,a)\,\delta(y - m\,c)$$

The above notation is too cumbersome, so we write it in a simpler way as:

$$f(\vec{r}) = \sum_j \delta^2\left(\vec{r} - \vec{R}_j\right) \longrightarrow$$ The summation over "j" is over all the lattice points

A 2D delta function has the property: $\int d^2\vec{r}\;\; \delta^2(\vec{r} - \vec{r}_o)\, g(\vec{r}) = g(\vec{r}_o)$
and it is just a product of two 1D delta functions corresponding to the x and y components of the vectors in its arguments: $\delta^2(\vec{r} - \vec{r}_o) = \delta(x - \vec{r}_o.\hat{x})\delta(y - \vec{r}_o.\hat{y})$

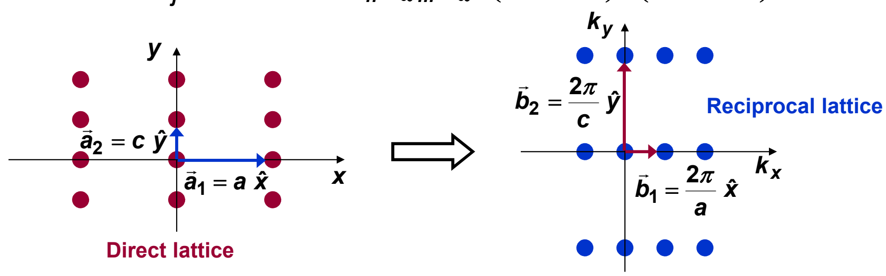
Now we Fourier transform the function $f(\vec{r})$:

$$f(\vec{k}) = \int d^2\vec{r}\;\; f(\vec{r})\; e^{-i\,\vec{k}\,.\,\vec{r}} = \int d^2\vec{r}\;\; \sum_j \delta^2\left(\vec{r} - \vec{R}_j\right)\, e^{-i\,\vec{k}\,.\,\vec{r}}$$

$$= \sum_j e^{-i\,\vec{k}\,.\,\vec{R}_j} = \frac{(2\pi)^2}{ac} \sum_{n=-\infty}^{\infty}\sum_{m=-\infty}^{\infty} \delta\left(k_x - n\frac{2\pi}{a}\right)\delta\left(k_y - m\frac{2\pi}{c}\right)$$

Reciprocal Lattice of a 2D Lattice

$$f(\vec{k}) = \sum_j e^{-i\,\vec{k}\,.\,\vec{R}_j} = \frac{(2\pi)^2}{ac} \sum_{n=-\infty}^{\infty} \sum_{m=-\infty}^{\infty} \delta\left(k_x - n\frac{2\pi}{a}\right)\delta\left(k_y - m\frac{2\pi}{c}\right)$$



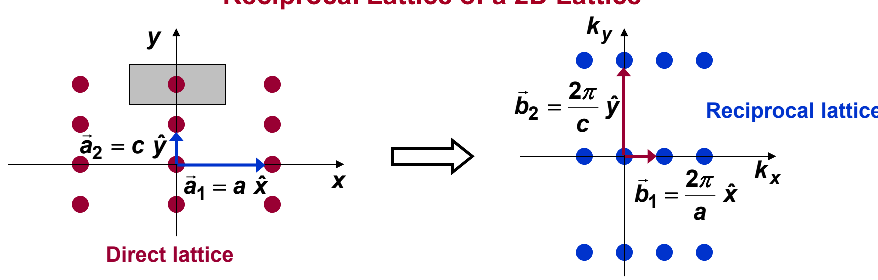
- Note also that the reciprocal lattice in k-space is defined by the set of all points for which the k-vector satisfies,

$$e^{i\,\vec{k}\,.\,\vec{R}_j} = 1$$

for all $\vec{R}_j$ of the direct lattice

- Reciprocal lattice as the FT of the direct lattice or as set of all points in k-space for which $\exp\left(i\,\vec{k}\,.\,\vec{R}_j\right) = 1$ for all $\vec{R}_j$, are equivalent statements

Reciprocal Lattice of a 2D Lattice



- The reciprocal lattice of a Bravais lattice is always a Bravais lattice and has its own primitive lattice vectors, for example, $\vec{b}_1$ and $\vec{b}_2$ in the above figure

- The position vector $\vec{G}$ of any point in the reciprocal lattice can be expressed in terms of the primitive lattice vectors:

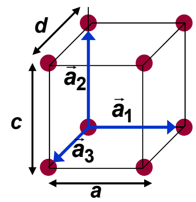
$$\vec{G} = n\,\vec{b}_1 + m\,\vec{b}_2 \quad \Big\{ \text{For } m \text{ and } n \text{ integers}$$

So we can write the FT in a better way as:

$$f(\vec{k}) = \frac{(2\pi)^2}{ac} \sum_{n=-\infty}^{\infty} \sum_{m=-\infty}^{\infty} \delta\left(k_x - n\frac{2\pi}{a}\right)\delta\left(k_y - m\frac{2\pi}{c}\right) = \frac{(2\pi)^2}{\Omega_2} \sum_j \delta^2\left(\vec{k} - \vec{G}_j\right)$$

where $\Omega_2 = ac$ is the area of the direct lattice primitive cell

Reciprocal Lattice of a 3D Lattice



Consider a orthorhombic direct lattice:

$$\vec{R} = n\,\vec{a}_1 + m\,\vec{a}_2 + p\,\vec{a}_3 \qquad \text{where } n,\ m, \text{ and } p \text{ are integers}$$

Then the corresponding delta-function lattice is:

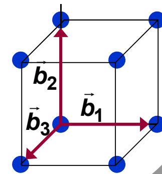
$$f(\vec{r}) = \sum_j \delta^3\left(\vec{r} - \vec{R}_j\right)$$

A 3D delta function has the property: $\int d^3\vec{r}\ \ \delta^3(\vec{r} - \vec{r}_o)\, g(\vec{r}) = g(\vec{r}_o)$

The reciprocal lattice in k-space is defined by the set of all points for which the k-vector satisfies: $\exp\left(i\,\vec{k}\,.\,\vec{R}_j\right) = 1$ for all $\vec{R}_j$ of the direct lattice. The above relation will hold if $\vec{k}$ equals $\vec{G}$:

$$\vec{G} = n\,\vec{b}_1 + m\,\vec{b}_2 + p\,\vec{b}_3 \qquad \text{and} \qquad \vec{b}_1 = \frac{2\pi}{a}\,\hat{x} \qquad \vec{b}_2 = \frac{2\pi}{c}\,\hat{y} \qquad \vec{b}_3 = \frac{2\pi}{d}\,\hat{z}$$

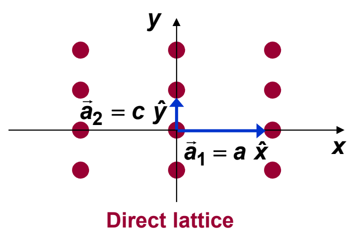
Finally, the FT of the direct lattice is:

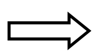


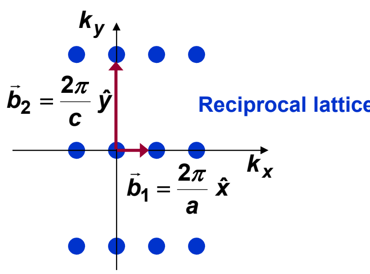
$$f(\vec{k}) = \int d^3\vec{r}\ \ f(\vec{r})\ e^{-i\,\vec{k}\,.\,\vec{r}} = \int d^3\vec{r}\ \ \sum_j \delta^3\left(\vec{r} - \vec{R}_j\right)\ e^{-i\,\vec{k}\,.\,\vec{r}}$$

$$= \sum_j e^{-i\,\vec{k}\,.\,\vec{R}_j} = \frac{(2\pi)^3}{acd} \sum_j \delta^3\left(\vec{k} - \vec{G}_j\right) = \frac{(2\pi)^3}{\Omega_3} \sum_j \delta^3\left(\vec{k} - \vec{G}_j\right)$$

Direct Lattice Vectors and Reciprocal Lattice Vectors







$$\vec{R} = n\,\vec{a}_1 + m\,\vec{a}_2 \qquad\qquad \vec{G} = n\,\vec{b}_1 + m\,\vec{b}_2$$

Remember that the reciprocal lattice in k-space is defined by the set of all points for which the k-vector satisfies,

$$e^{i\,\vec{k}\,.\,\vec{R}} = 1$$

for all $\vec{R}$ of the direct lattice

So for all direct lattice vectors $\vec{R}$ and all reciprocal lattice vectors $\vec{G}$ we must have:

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

Reciprocal Lattice of General Lattices in 1D, 2D, 3D

More often that not, the direct lattice primitive vectors, $\vec{a}_1, \vec{a}_2$, and $\vec{a}_3$, are not orthogonal

Question: How does one find the reciprocal lattice vectors in the general case?

ID lattice:

If the direct lattice primitive vector is: $\vec{a}_1 = a\,\hat{x}$
and length of primitive cell is: $\Omega_1 = a$
Then the reciprocal lattice primitive vector is: $\vec{b}_1 = \dfrac{2\pi}{a}\,\hat{x}$

$$f(\vec{r}) = \sum_j \delta(\vec{r} - \vec{R}_j) \iff f(\vec{k}) = \frac{2\pi}{\Omega_1}\sum_j \delta(\vec{k} - \vec{G}_j)$$

Note:

$$\vec{a}_1 \cdot \vec{b}_1 = 2\pi$$

$$e^{i\,\vec{G}_p \cdot \vec{R}_m} = 1$$

2D lattice:

If the direct lattice is in the *x-y* plane and the primitive vectors are: $\vec{a}_1$ and $\vec{a}_2$
and area of primitive cell is: $\Omega_2 = |\vec{a}_1 \times \vec{a}_2|$
Then the reciprocal lattice primitive vectors are: $\vec{b}_1 = 2\pi\dfrac{\hat{a}_2 \times \hat{z}}{\Omega_2}$ $\quad \vec{b}_2 = 2\pi\dfrac{\hat{z} \times \hat{a}_1}{\Omega_2}$

$$f(\vec{r}) = \sum_j \delta^2(\vec{r} - \vec{R}_j) \iff f(\vec{k}) = \frac{(2\pi)^2}{\Omega_2}\sum_j \delta^2(\vec{k} - \vec{G}_j)$$

Note: $\vec{a}_j \cdot \vec{b}_k = 2\pi\,\delta_{jk}$ and $e^{i\,\vec{G}_p \cdot \vec{R}_m} = 1$

Reciprocal Lattice of General Lattices in 1D, 2D, 3D

3D lattice:

If the direct lattice primitive vectors are: $\vec{a}_1, \vec{a}_2$, and $\vec{a}_3$
and volume of primitive cell is: $\Omega_3 = |\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)|$

Then the reciprocal lattice primitive vectors are:

$$\vec{b}_1 = 2\pi\frac{\hat{a}_2 \times \hat{a}_3}{\Omega_3} \quad \vec{b}_2 = 2\pi\frac{\vec{a}_3 \times \vec{a}_1}{\Omega_3} \quad \vec{b}_3 = 2\pi\frac{\vec{a}_1 \times \vec{a}_2}{\Omega_3}$$

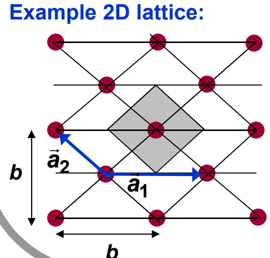
$$f(\vec{r}) = \sum_j \delta^3(\vec{r} - \vec{R}_j) \iff f(\vec{k}) = \frac{(2\pi)^3}{\Omega_3}\sum_j \delta^3(\vec{k} - \vec{G}_j)$$

Note:

$$\vec{a}_j \cdot \vec{b}_k = 2\pi\,\delta_{jk}$$

$$e^{i\,\vec{G}_p \cdot \vec{R}_m} = 1$$

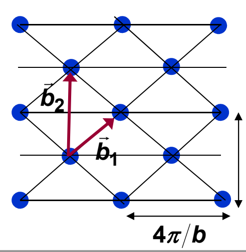
Example 2D lattice:



$$\vec{a}_1 = b\,\hat{x}$$

$$\vec{a}_2 = -\frac{b}{2}\,\hat{x} + \frac{b}{2}\,\hat{y}$$

$$\Omega_2 = |\vec{a}_1 \times \vec{a}_2| = \frac{b^2}{2}$$

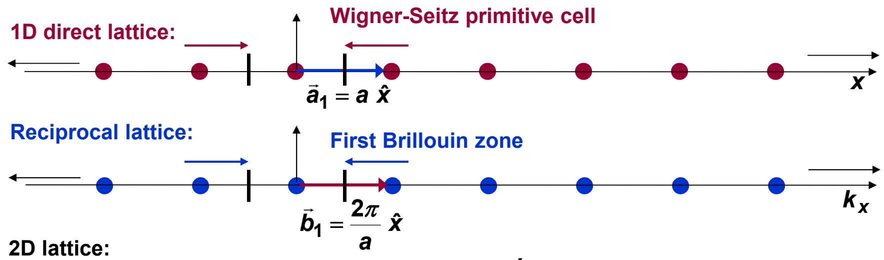


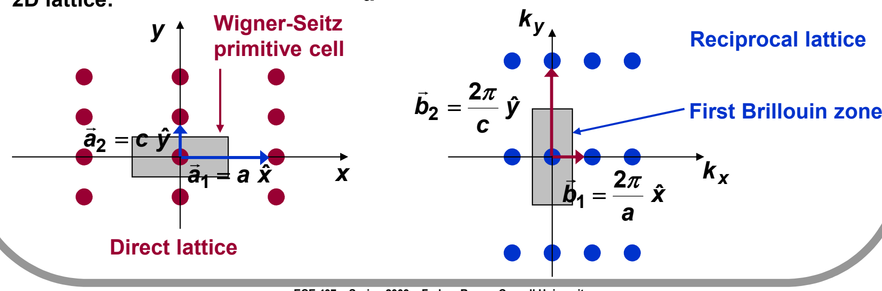
$$\vec{b}_1 = \frac{2\pi}{b}(\hat{x} + \hat{y})$$

$$\vec{b}_2 = \frac{4\pi}{b}\,\hat{y}$$

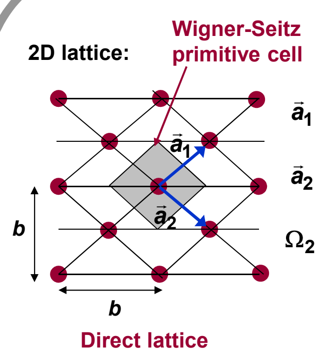
The Brillouin Zone

The Wigner-Seitz primitive cell of the reciprocal lattice centered at the origin is called the Brillouin zone (or the first Brillouin zone or FBZ)





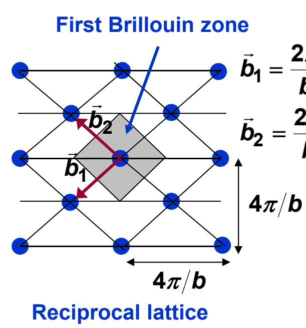
The Brillouin Zone



$$\vec{a}_1 = \frac{b}{2}\,\hat{x} + \frac{b}{2}\,\hat{y}$$

$$\vec{a}_2 = \frac{b}{2}\,\hat{x} - \frac{b}{2}\,\hat{y}$$

$$\Omega_2 = \left|\vec{a}_1 \times \vec{a}_2\right| = \frac{b^2}{2}$$



$$\vec{b}_1 = \frac{2\pi}{b}\left(-\hat{x} - \hat{y}\right)$$

$$\vec{b}_2 = \frac{2\pi}{b}\left(-\hat{x} + \hat{y}\right)$$

Volume/Area/Length of the first Brillouin zone:

The volume (3D), area (2D), length (1D) of the first Brillouin zone is given in the same way as the corresponding expressions for the primitive cell of a direct lattice:

1D $\quad \Pi_1 = \left|\vec{b}_1\right|$

2D $\quad \Pi_2 = \left|\vec{b}_1 \times \vec{b}_2\right|$

3D $\quad \Pi_3 = \left|\vec{b}_1 \cdot \left(\vec{b}_2 \times \vec{b}_3\right)\right|$

Note that in all dimensions (d) the following relationship holds between the volumes, areas, lengths of the direct and reciprocal lattice primitive cells:

$$\Pi_d = \frac{(2\pi)^d}{\Omega_d}$$

ECE 407 – Spring 2009 – Farhan Rana – Cornell University

Direct Lattice Planes and Reciprocal Lattice Vectors

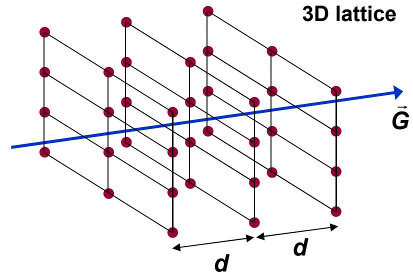
There is an intimate relationship between reciprocal lattice vectors and planes of points in the direct lattice captured by this theorem and its converse

Theorem:
If there is a family of parallel lattice planes separated by distance "d" and $\hat{n}$ is a unit vector normal to the planes then the vector given by,

$$\vec{G} = \frac{2\pi}{d}\,\hat{n}$$

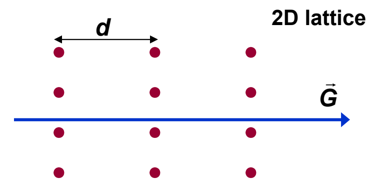
is a reciprocal lattice vector and so is:

$$m\frac{2\pi}{d}\,\hat{n} \qquad \{ \quad m = \text{integer}$$

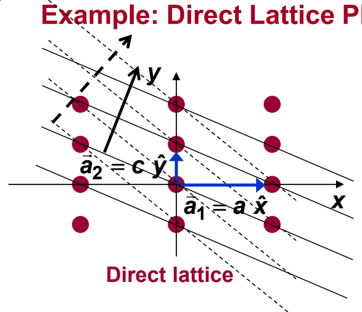


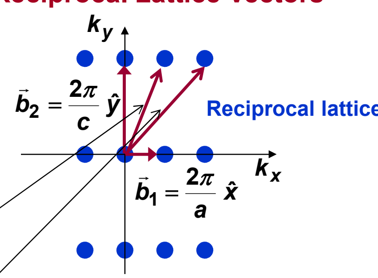
Converse:
If $\vec{G}_1$ is any reciprocal lattice vector, and $\vec{G}$ is the reciprocal lattice vector of the smallest magnitude parallel to $\vec{G}_1$, then there exist a family of lattice planes perpendicular to $\vec{G}_1$ and $\vec{G}$, and separated by distance "d" where:

$$d = \frac{2\pi}{|\vec{G}|}$$



Example: Direct Lattice Planes and Reciprocal Lattice Vectors





Consider:

$$\vec{G} = \vec{b}_1 + \vec{b}_2 = 2\pi\left(\frac{\hat{x}}{a} + \frac{\hat{y}}{c}\right)$$

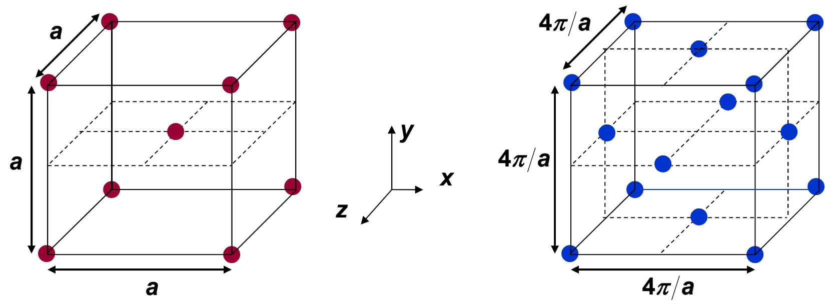
There must be a family of lattice planes normal to $\vec{G}$ and separated by: $\dfrac{2\pi}{|\vec{G}|} = \dfrac{ac}{\sqrt{a^2 + c^2}}$

Now consider:

$$\vec{G} = 2\vec{b}_1 + \vec{b}_2 = 2\pi\left(\frac{2\hat{x}}{a} + \frac{\hat{y}}{c}\right)$$

There must be a family of lattice planes normal to $\vec{G}$ and separated by: $\dfrac{2\pi}{|\vec{G}|} = \dfrac{ac}{\sqrt{a^2 + 4c^2}}$

The BCC Direct Lattice



Direct lattice: BCC

Reciprocal lattice: FCC

The direct and the reciprocal lattices are not necessarily always the same!

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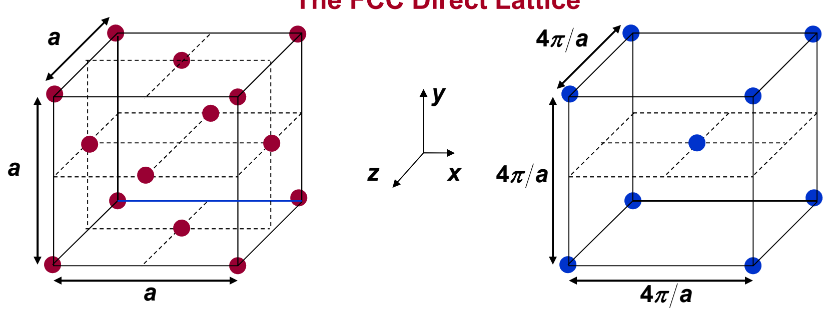
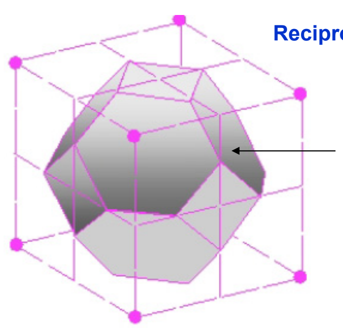
The FCC Direct Lattice



Direct lattice: FCC

Reciprocal lattice: BCC



First Brillouin zone of the BCC reciprocal lattice for an FCC direct lattice

The Reciprocal Lattice and FTs of Periodic Functions

The relationship between delta-functions on a "*d*" dimensional lattice and its Fourier transform is:

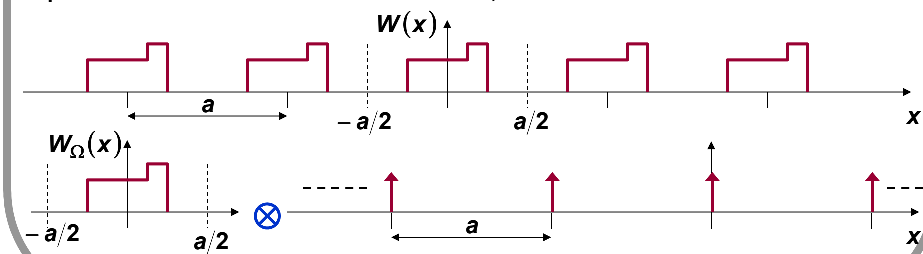
$$f(\vec{r}) = \sum_j \delta^d\left(\vec{r} - \vec{R}_j\right) \iff f(\vec{k}) = \frac{(2\pi)^d}{\Omega_d} \sum_j \delta^d\left(\vec{k} - \vec{G}_j\right)$$

Supper $W(\vec{r})$ is a periodic function with the periodicity of the direct lattice then by definition:

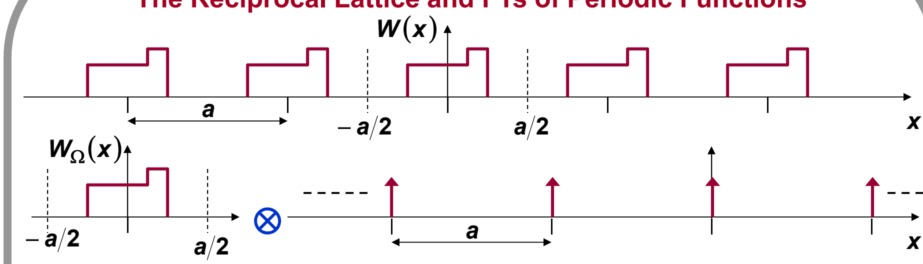
$$W\left(\vec{r} + \vec{R}_j\right) = W(\vec{r})$$

for all $\vec{R}_j$ of the direct lattice

One can always write a periodic function as a convolution of its value in the primitive cell and a lattice of delta functions, as shown for 1D below:



The Reciprocal Lattice and FTs of Periodic Functions



Mathematically:

$$W(x) = W_\Omega(x) \otimes \sum_{n=-\infty}^{\infty} \delta(x - n\,a)$$

And more generally in "*d*" dimensions for a lattice periodic function $W(\vec{r})$ we have:

$$W(\vec{r}) = W_\Omega(\vec{r}) \otimes \sum_j \delta^d\left(\vec{r} - \vec{R}_j\right)$$

Value of the function in one primitive cell

Lattice of delta functions

The Reciprocal Lattice and FTs of Periodic Functions

For a periodic function we have:

$$W(\vec{r}) = W_\Omega(\vec{r}) \otimes \sum_j \delta^d(\vec{r} - \vec{R}_j)$$

Its FT is now easy given that we know the FT of a lattice of delta functions:

$$f(\vec{r}) = \sum_j \delta^d(\vec{r} - \vec{R}_j) \iff f(\vec{k}) = \frac{(2\pi)^d}{\Omega_d} \sum_j \delta^d(\vec{k} - \vec{G}_j)$$

We get:

$$W(\vec{k}) = W_\Omega(\vec{k}) \times \frac{(2\pi)^d}{\Omega_d} \sum_j \delta^d(\vec{k} - \vec{G}_j) = \frac{(2\pi)^d}{\Omega_d} \sum_j \delta^d(\vec{k} - \vec{G}_j) W_\Omega(\vec{G}_j)$$

The FT looks like reciprocal lattice of delta-functions with unequal weights

If we now take the inverse FT we get:

$$W(\vec{r}) = \int \frac{d^d\vec{k}}{(2\pi)^d} W(\vec{k}) e^{i\vec{k}\cdot\vec{r}} = \int \frac{d^d\vec{k}}{(2\pi)^d} \frac{(2\pi)^d}{\Omega_d} \sum_j \delta^d(\vec{k} - \vec{G}_j) W_\Omega(\vec{G}_j) e^{i\vec{k}\cdot\vec{r}}$$

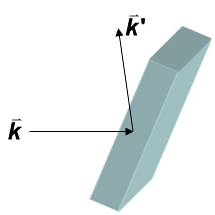
$$= \sum_j \frac{W_\Omega(\vec{G}_j)}{\Omega_d} e^{i\vec{G}_j\cdot\vec{r}}$$

A lattice periodic function can always be written as a Fourier series that only has wavevectors belonging to the reciprocal lattice

The Reciprocal Lattice and X-Ray Diffraction

X-ray diffraction is the most commonly used method to study crystal structures

In this scheme, X-rays of wavevector $\vec{k}$ are sent into a crystal, and the scattered X-rays in the direction of a different wavevector, say $\vec{k}'$, are measured



If the position dependent dielectric constant of the medium is given by $\varepsilon(\vec{r})$ then the diffraction theory tells us that the amplitude of the scattered X-rays in the direction of $\vec{k}'$ is proportional to the integral:

$$S(\vec{k} \to \vec{k}') \propto \int d^3\vec{r}\; e^{-i\vec{k}'\cdot\vec{r}}\, \varepsilon(\vec{r})\, e^{i\vec{k}\cdot\vec{r}}$$

For X-ray frequencies, the dielectric constant is a periodic function with the periodicity of the lattice. Therefore, one can write:

$$\varepsilon(\vec{r}) = \sum_j \varepsilon(\vec{G}_j) e^{i\vec{G}_j\cdot\vec{r}}$$

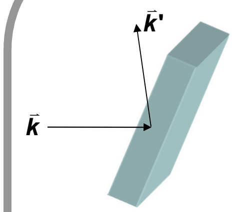
Plug this into the integral above to get: $S(\vec{k} \to \vec{k}') \propto \sum_j \varepsilon(\vec{G}_j)(2\pi)^3 \delta(\vec{k} + \vec{G}_j - \vec{k}')$

$\Rightarrow$ X-rays will scatter in only those directions for which:

$\vec{k}' = \vec{k} + \vec{G}$ where $\vec{G}$ is some reciprocal lattice vector

Or: $\vec{k}' = \vec{k} \pm \vec{G}$ Because $-\vec{G}$ is also a reciprocal vector whenever $\vec{G}$ is a reciprocal vector

The Reciprocal Lattice and X-Ray Diffraction



$\Rightarrow$ X-rays will scatter in only those directions for which:

$$\vec{k}' = \vec{k} \pm \vec{G} \qquad \longrightarrow (1)$$

Also, the frequency of the incident and diffracted X-rays is the same so:

$$\omega' = \omega$$

$$\Rightarrow |\vec{k}'| c = |\vec{k}| c$$

$$\Rightarrow |\vec{k}'| = |\vec{k}|$$

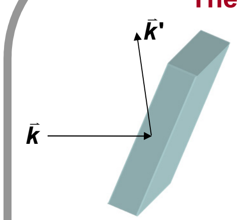
(1) gives: $|\vec{k}'|^2 = |\vec{k}|^2 + |\vec{G}|^2 \pm 2\,\vec{k}\,.\,\vec{G}$

$$\Rightarrow |\vec{k}'|^2 = |\vec{k}|^2 + |\vec{G}|^2 \pm 2\,\vec{k}\,.\,\vec{G}$$

$$\Rightarrow |\vec{k}|^2 = |\vec{k}|^2 + |\vec{G}|^2 \pm 2\,\vec{k}\,.\,\vec{G}$$

$$\Rightarrow \pm\,\vec{k}\,.\,\vec{G} = \frac{|\vec{G}|^2}{2} \quad \Big\{ \text{Condition for X-ray diffraction}$$

The Reciprocal Lattice and X-Ray Diffraction



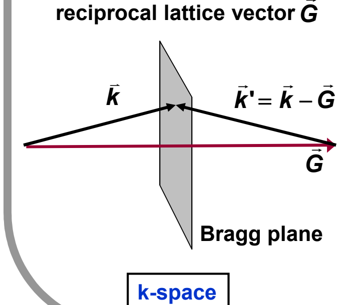
The condition,

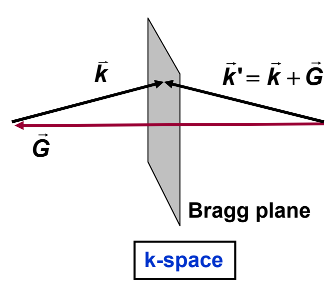
$$\vec{k}\,.\,\vec{G} = \pm\frac{|\vec{G}|^2}{2}$$

is called the Bragg condition for diffraction

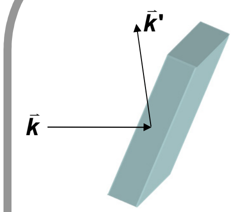
Incident X-rays will diffract efficiently provided the incident wavevector satisfies the Bragg condition for some reciprocal lattice vector $\vec{G}$

A graphical way to see the Bragg condition is that the incident wavevector lies on a plane in k-space (called the Bragg plane) that is the perpendicular bisector of some reciprocal lattice vector $\vec{G}$





The Reciprocal Lattice and X-Ray Diffraction



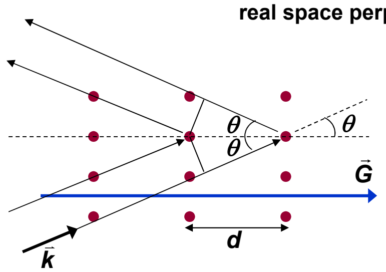
The condition,

$$\vec{k}\,.\,\vec{G} = \pm\frac{|\vec{G}|^2}{2}$$

can also be interpreted the following way:

Incident X-rays will diffract efficiently when the reflected waves from successive atomic planes add in phase

**Recall that there are always a family of lattice planes in real space perpendicular to any reciprocal lattice vector



Real space

$$\vec{G} = m\frac{2\pi}{d}\hat{n}$$

Condition for in-phase reflection from successive lattice planes:

$$2d\cos(\theta) = m\,\lambda$$

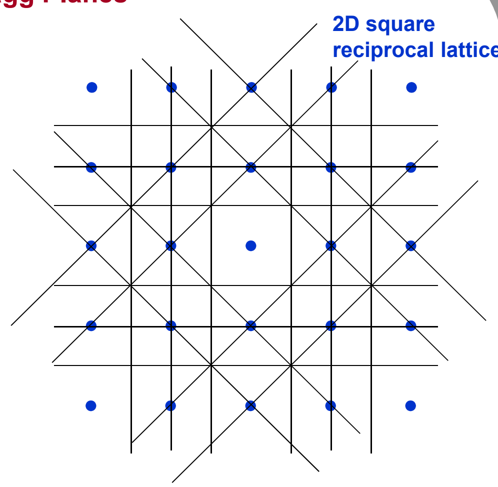
$$\Rightarrow \frac{2\pi}{\lambda}\left(m\frac{2\pi}{d}\right)\cos(\theta) = \frac{1}{2}\left(m\frac{2\pi}{d}\right)^2$$

$$\Rightarrow \vec{k}\,.\,\vec{G} = \frac{|\vec{G}|^2}{2}$$

Bragg Planes

Corresponding to every reciprocal lattice vector there is a Bragg plane in k-space that is a perpendicular bisector of that reciprocal lattice vector

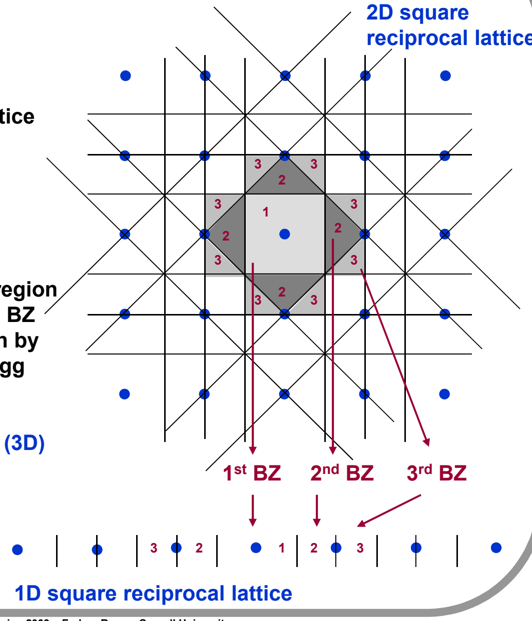
Lets draw few of the Bragg planes for the square 2D reciprocal lattice corresponding to the reciprocal lattice vectors of the smallest magnitude



1D square reciprocal lattice

Bragg Planes and Higher Order Brillouin Zones

Bragg planes are shown for the square 2D reciprocal lattice corresponding to the reciprocal lattice vectors of the smallest magnitude



Higher Order Brillouin Zones

The nth BZ can be defined as the region in k-space that is not in the (n-1)th BZ and can be reached from the origin by crossing at the minimum (n-1) Bragg planes

The length (1D), area (2D), volume (3D) of BZ of any order is the same

Appendix: Proof of the General Lattice FT Relation in 3D

This appendix gives proof of the FT relation:

$$f(\vec{r}) = \sum_j \delta^3(\vec{r}-\vec{R}_j) \quad \Longleftrightarrow \quad f(\vec{k}) = \frac{(2\pi)^3}{\Omega_3} \sum_j \delta^3(\vec{k}-\vec{G}_j)$$

for the general case when the direct lattice primitive vectors are not orthogonal

Let: $\vec{R} = n_1\,\vec{a}_1 + n_2\,\vec{a}_2 + n_3\,\vec{a}_3$

Define the reciprocal lattice primitive vectors as:

$$\vec{b}_1 = 2\pi\frac{\vec{a}_2\times\vec{a}_3}{\Omega_3} \qquad \vec{b}_2 = 2\pi\frac{\vec{a}_3\times\vec{a}_1}{\Omega_3} \qquad \vec{b}_3 = 2\pi\frac{\vec{a}_1\times\vec{a}_2}{\Omega_3}$$

Note: $\vec{a}_j\,.\,\vec{b}_k = 2\pi\,\delta_{jk}$

Now we take FT:

$$f(\vec{k}) = \int d^3\vec{r}\;\; f(\vec{r})\; e^{-i\,\vec{k}\,.\,\vec{r}} = \int d^3\vec{r}\;\; \sum_j \delta^3(\vec{r}-\vec{R}_j)\; e^{-i\,\vec{k}\,.\,\vec{r}}$$

$$= \sum_j e^{-i\,\vec{k}\,.\,\vec{R}_j}$$

Appendix: Proof

One can expand $\vec{k}$ in any suitable basis. Instead of choosing the usual basis:

$$\vec{k} = k_x \hat{x} + k_y \hat{y} + k_z \hat{z}$$

I choose the basis defined by the reciprocal lattice primitive vectors:

$$\vec{k} = k_1\, \vec{b}_1 + k_2\, \vec{b}_2 + k_3\, \vec{b}_3$$

Given that: $\vec{a}_j \,.\, \vec{b}_k = 2\pi\, \delta_{jk}$

I get:

$$f(\vec{k}) = \sum_j e^{-i\,\vec{k}\,.\,\vec{R}_j} = \sum_{n_1\, n_2\, n_3} e^{-i\,\vec{k}\,.\,(n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3)}$$

$$= \sum_{m_1\, m_2\, m_3} \delta(k_1 - m_1)\, \delta(k_2 - m_2)\, \delta(k_3 - m_3)$$

Now:

$$\delta(k_1 - m_1)\, \delta(k_2 - m_2)\, \delta(k_3 - m_3) \propto \delta^3(\vec{k} - \vec{G})$$

where: $\vec{G} = m_1\, \vec{b}_1 + m_2\, \vec{b}_2 + m_3\, \vec{b}_3$

But we don't know the exact weight of the delta function $\delta^3(\vec{k} - \vec{G})$

Appendix: Proof

Since: $\vec{k} = k_x \hat{x} + k_y \hat{y} + k_z \hat{z}$ and $\vec{k} = k_1\, \vec{b}_1 + k_2\, \vec{b}_2 + k_3\, \vec{b}_3$

This implies:

$$\begin{bmatrix} k_x \\ k_y \\ k_z \end{bmatrix} = \begin{bmatrix} b_{1x} & b_{2x} & b_{3x} \\ b_{2x} & b_{2y} & b_{2z} \\ b_{3x} & b_{3y} & b_{3z} \end{bmatrix} \begin{bmatrix} k_1 \\ k_2 \\ k_3 \end{bmatrix} \qquad \text{———— (1)}$$

Any integral over k-space in the form: $\int_{-\infty}^{\infty} dk_1 \int_{-\infty}^{\infty} dk_2 \int_{-\infty}^{\infty} dk_3$

can be converted into an integral in the form: $\int_{-\infty}^{\infty} dk_x \int_{-\infty}^{\infty} dk_y \int_{-\infty}^{\infty} dk_z$

by the Jacobian of the transformation:

$$\int_{-\infty}^{\infty} dk_x \int_{-\infty}^{\infty} dk_y \int_{-\infty}^{\infty} dk_z \;\to\; \left| \frac{\partial(k_x\,,k_y\,,k_z)}{\partial(k_1\,,k_2\,,k_3)} \right| \int_{-\infty}^{\infty} dk_1 \int_{-\infty}^{\infty} dk_2 \int_{-\infty}^{\infty} dk_3$$

Therefore:

$$\delta(k_1 - m_1)\, \delta(k_2 - m_2)\, \delta(k_3 - m_3) = \left| \frac{\partial(k_x,k_y,k_z)}{\partial(k_1,k_2,k_3)} \right| \delta^3(\vec{k} - \vec{G})$$

Appendix: Proof

From (1) on previous slide:

$$\left|\frac{\partial(k_x, k_y, k_z)}{\partial(k_1, k_2, k_3)}\right| = \left|\vec{b}_1 \,.\, (\vec{b}_2 \times \vec{b}_3)\right| = \Pi_3 = \frac{(2\pi)^3}{\Omega_3}$$

Therefore:

$$f(\vec{k}) = \sum_j e^{-i\,\vec{k}\,.\,\vec{R}_j} = \sum_{m_1\, m_2\, m_3} \delta(k_1 - m_1)\,\delta(k_2 - m_2)\,\delta(k_3 - m_3)$$

$$= \frac{(2\pi)^3}{\Omega_3} \sum_j \delta^3\left(\vec{k} - \vec{G}_j\right)$$