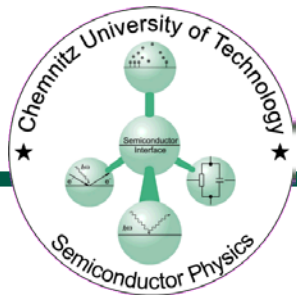




# THE RECIPROCAL SPACE & THE FOURIER TRANSFORM



## What's the purpose of studying the Reciprocal Lattice?

The **Reciprocal Space** is the most convenient space for calculation of **solid state properties** and **electronic structure**. (You can do these calculations in the direct space as well but the calculations would be more difficult.)

The reciprocal lattice plays a fundamental role in most **analytic studies of periodic structures**, particularly in the theory of diffraction.

The **diffraction pattern of a crystal** can be used to **determine the reciprocal vectors of the lattice**. Using this process, one can **infer the atomic arrangement of a crystal**.

# The Reciprocal Lattice

In physics, the **reciprocal lattice** represents the **Fourier transform** of a *direct lattice*.

The **recipocal lattices** exist in the **reciprocal space** also called the **momentum space** or the **K-space**.

The **direct lattices** exist in **real space**.

The **Bravais Lattices** are **direct lattices**  
BUT  
the **reciprocal lattice** is also a **Bravais Lattice**

# What is a Fourier Transform?

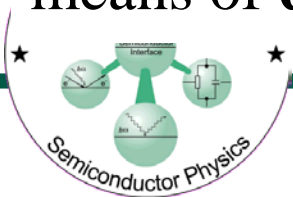
## Why do we define the reciprocal lattice using these transforms?

The **key feature of crystals** is their **periodicity** ; this property will be utilised very often when describing the underlying physics.

Accordingly, the physics that occurs within a crystal will reflect this periodicity as well.

From this general consideration one can already guess that an aspect closely related with the description of crystals will be the topic of mechanical/electromagnetic waves due to their periodic nature.

A concrete example for this is the **structure determination** by means of **diffraction**.



## CRYSTAL

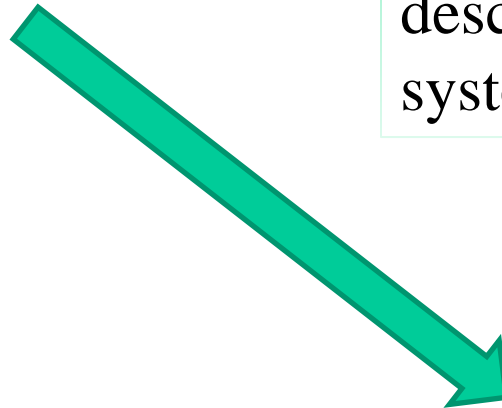
Periodic Structure in Space



Physical phenomena  
Dominated, regulated  
by a periodic structure

## Fourier Series

Mathematical function that  
describes Periodic physical  
systems.



## Fourier Transforms



## ➡ Fourier Analysis of a crystal structure

RECALL; A Fourier series is an expansion of a periodic function in terms of an infinite sum of **sines** and **cosines**.

By introducing more and more sine and cosine functions of different frequencies the Fourier series approaches the original function.

Consider the 1D function  $f(x)$  with a period  $a$  i.e.  $f(x) = f(x+a)$   
This function can be expanded in a Fourier series as;

$$f(x) = f_0 + \sum_{p=1}^{\infty} C_p \cos\left(\frac{2\pi p x}{a}\right) + \sum_{p=1}^{\infty} S_p \sin\left(\frac{2\pi p x}{a}\right)$$

OR 
$$f(x) = \sum_p f_p e^{(i 2\pi p x / a)}$$

Where  $p$  are positive integers,  $C_p$   $S_p$  are the Fourier coefficients of the expansion and  $f_p$  are the complex coefficients

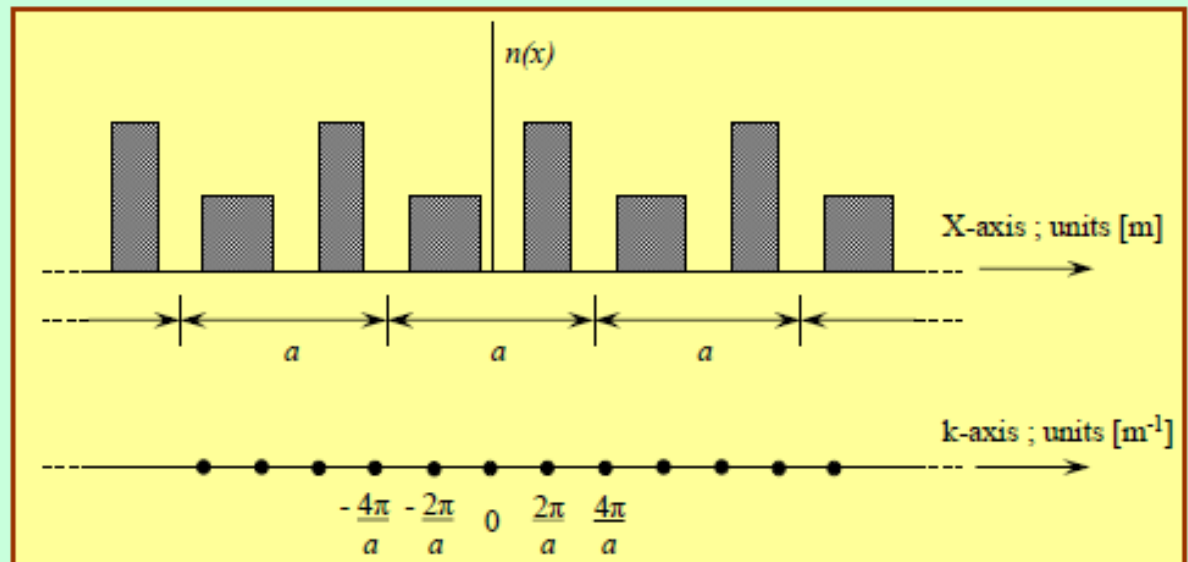
## ➡ Fourier Analysis of a crystal structure

$$n(x) = \sum_p n_p e^{(i2\pi p x/a)}$$

We say that  $\frac{2\pi p}{a}$  forms a set of points in the 1D reciprocal lattice of the crystal.

For a 1D crystal the reciprocal lattice is a line of points separated by  $2\pi/a$ . The reciprocal lattice points tell us the allowed terms in the Fourier series. A term is allowed if it is consistent with the periodicity of the crystal.

A periodic function  $n(x)$  of period  $a$ , and the terms  $2\pi p/a$  that may appear in the Fourier transform of  $n(x)$



## ➡ Real Space and Reciprocal Space

We now introduce the concepts of real and reciprocal space.

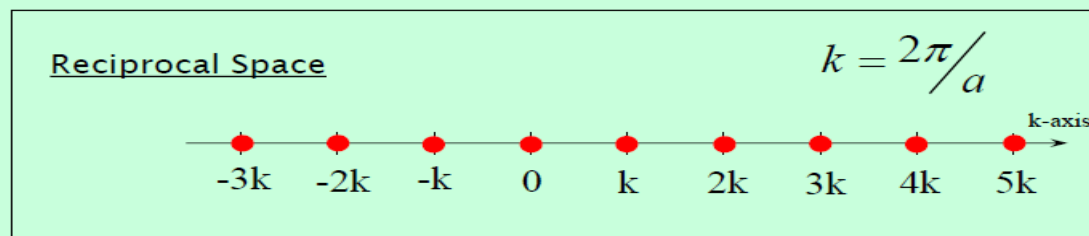
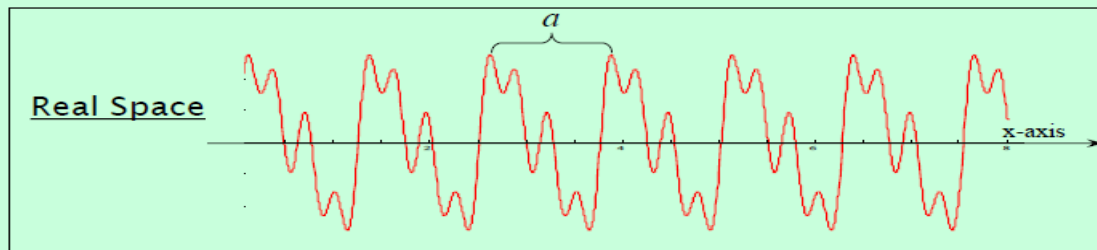
**Reciprocal Space:** Is also called k-space and is the space in which the Fourier transform of a spatial function is represented.

A Fourier transform will take us from real space to reciprocal space and vice versa.

It is beneficial to make certain observations

### ➡ General function in Real and Reciprocal space

Consider a more general periodic function  $n(x+a) = n(x)$





## ➡ Fourier Analysis of a crystal structure

Consider first a 1D crystal lattice described by a function  $n(x)$  with period  $a$  in the  $x$ -direction and expand its Fourier series to get;

$$n(x) = n_0 + \sum_{p=1}^{\infty} C_p \cos\left(\frac{2\pi p x}{a}\right) + \sum_{p=1}^{\infty} S_p \sin\left(\frac{2\pi p x}{a}\right)$$

To show that this still retains the periodicity of the original function sub in  $(x + a)$  to get;

$$\begin{aligned} n(x+a) &= n_0 + \sum_{p=1}^{\infty} C_p \cos\left(\frac{2\pi p x}{a} + 2\pi p\right) + \sum_{p=1}^{\infty} S_p \sin\left(\frac{2\pi p x}{a} + 2\pi p\right) \\ &= n_0 + \sum_{p=1}^{\infty} C_p \cos\left(\frac{2\pi p x}{a}\right) + \sum_{p=1}^{\infty} S_p \sin\left(\frac{2\pi p x}{a}\right) \\ &= n(x) \end{aligned}$$

Should apply equally to the 3 directions in space.

## ➡ Fourier Analysis of a crystal structure

When dealing with a crystal structure, due to its underlying Bravais lattice, we know that it is invariant under any translation of the form;

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

where  $u_1$   $u_2$   $u_3$  are integers and  $\mathbf{a}_1$   $\mathbf{a}_2$   $\mathbf{a}_3$  are the primitive vectors

And so local physical properties of the crystal can be described using periodic functions.

For example the electron number density  $n(\mathbf{r})$  is a periodic function of  $\mathbf{r}$ , with periods  $\mathbf{a}_1$  ;  $\mathbf{a}_2$  ;  $\mathbf{a}_3$  in the directions of the three crystal axes, respectively and

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

## ➡ Reciprocal Lattice

The two lattices are related by;

$$\mathbf{b}_1 = 2\pi \frac{\mathbf{a}_2 \times \mathbf{a}_3}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)}; \quad \mathbf{b}_2 = 2\pi \frac{\mathbf{a}_3 \times \mathbf{a}_1}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)}; \quad \mathbf{b}_3 = 2\pi \frac{\mathbf{a}_1 \times \mathbf{a}_2}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)}$$

Where  $\mathbf{a}_1; \mathbf{a}_2; \mathbf{a}_3$  are the primitive vectors of the **bravais** lattice and  $\mathbf{b}_1; \mathbf{b}_2; \mathbf{b}_3$  are the primitive vectors of the **reciprocal** lattice.

Notice that:

- $\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3) = V$  the volume of the unit cell in real space;
- $\mathbf{b}_1, \mathbf{b}_2, \mathbf{b}_3$  are the result of a cross product between 2 primitive vectors of the direct lattice, which implies they are perpendicular to each other;
- The magnitude/ size of any primitive vector in the reciprocal lattice will be reciprocally proportional to the ones in the direct lattice and vice versa because :  $\mathbf{a}_i \cdot \mathbf{b}_j = 2\pi\delta_{i,j}$  ( $i,j=1,2,3$ ); for  $i=j$   $\delta_{i,j} = 1$ ;  $\delta_{i,j} = 0$  for  $i \neq j$

# The reciprocal lattice is a Bravais lattice

## ➡ Reciprocal Lattice

### The reciprocal lattice is also a Bravais lattice (Proof 2)

Any vector,  $\mathbf{k}$ , in the reciprocal lattice can be written as a linear combination of the primitive vectors;

$$\bar{\mathbf{k}} = k_1 \bar{\mathbf{b}}_1 + k_2 \bar{\mathbf{b}}_2 + k_3 \bar{\mathbf{b}}_3$$

$$\text{where; } \bar{\mathbf{b}}_1 = 2\pi \frac{\mathbf{a}_2 \times \mathbf{a}_3}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)}; \quad \bar{\mathbf{b}}_2 = 2\pi \frac{\mathbf{a}_3 \times \mathbf{a}_1}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)}; \quad \bar{\mathbf{b}}_3 = 2\pi \frac{\mathbf{a}_1 \times \mathbf{a}_2}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)}; \quad k_i \in \mathbf{Z}$$

From this we can see that;  $\bar{\mathbf{b}}_i \cdot \bar{\mathbf{a}}_j = 2\pi \delta_{ij}$ ; where;  $\delta_{ij} = 0$  if  $i \neq j$   
 $\delta_{ij} = 1$  if  $i = j$

let  $\mathbf{R}$  be a vector in the direct lattice so;  $\bar{\mathbf{R}} = n_1 \bar{\mathbf{a}}_1 + n_2 \bar{\mathbf{a}}_2 + n_3 \bar{\mathbf{a}}_3$   $n_i \in \mathbf{Z}$

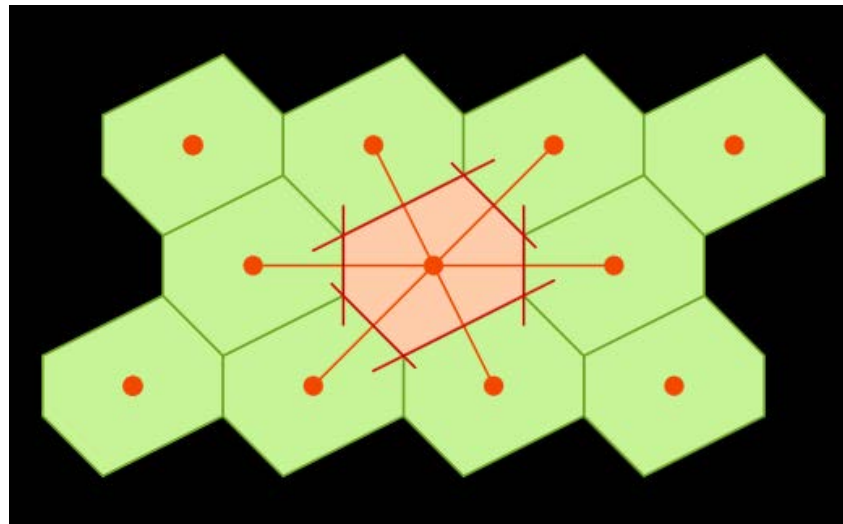
$$\text{and; } \bar{\mathbf{k}} \cdot \bar{\mathbf{R}} = 2\pi(k_1 n_1 + k_2 n_2 + k_3 n_3)$$

From the definition of a reciprocal lattice vector  $\mathbf{k}$  must satisfy  $e^{i\bar{\mathbf{k}} \cdot \bar{\mathbf{R}}} = 1$   
In order for this to be true  $\bar{\mathbf{k}} \cdot \bar{\mathbf{R}}$  must equal  $2\pi$  times an integer.  
This is fulfilled as  $n_i \in \mathbf{Z}$  and  $k_i \in \mathbf{Z}$  and so the reciprocal lattice is also a Bravais lattice.

# The Wigner-Seitz Cell

Special type of primitive-cells.

The *Wigner-Seitz cell* of a lattice point is defined as the **volume** that encloses all points in space which are closer to this particular **lattice point** than to any other.



**Bcc**

**Fcc**

## Construction

1<sup>st</sup> step: Choose any lattice point and draw connecting lines to its closest neighbours.

2<sup>nd</sup> step: Draw the perpendicular bisectors of the connecting lines.

Final result: The enclosed area defined by the intersection of this connecting lines is the Wigner-Seitz cell. It forms a unit cell, i.e. is able to build the whole lattice without gaps/overlaps.

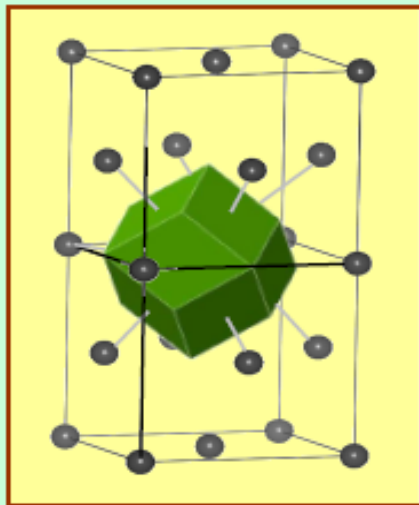


# Examples of Bravais Lattices in the Reciprocal Space

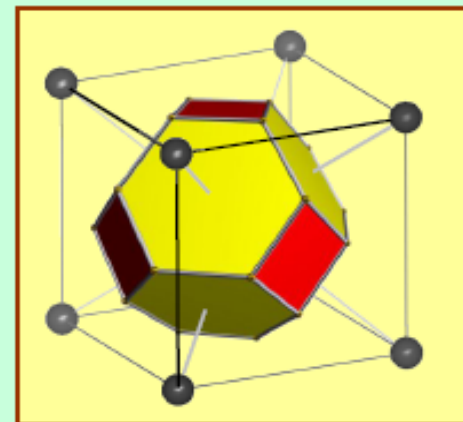
## ➡ Reciprocal Lattice primitive cell

If the volume of the primitive cell in the *direct lattice* is given by  $V$ , then the volume of the primitive cell of the *reciprocal lattice* is  $\frac{(2\pi)^3}{V}$

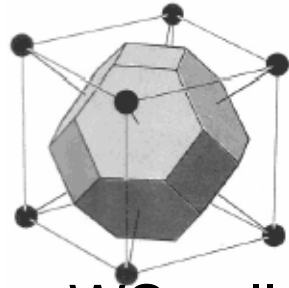
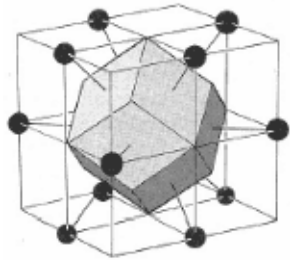
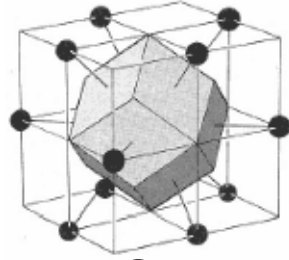
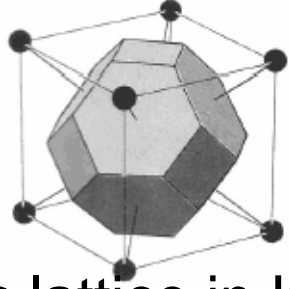
The Wigner-Seitz primitive cell of the *reciprocal lattice* is known as the first Brillouin Zone.



The first Brillouin Zone for the BCC lattice



The first Brillouin Zone for the FCC lattice

| Lattice Real Space   | Lattice K-space  |
|--|--|
|  <p>bcc WS cell</p> |  <p>bcc BZ (fcc lattice in K-space)</p> |
|  <p>fcc WS cell</p> |  <p>fcc BZ (bcc lattice in K-space)</p> |

- ✓ The WS cell of bcc lattice in real space transforms to a Brillouin zone (BZ) in a fcc lattice in reciprocal space;
- ✓ The WS cell of a fcc lattice transforms to a Brillouin zone of a bcc lattice in reciprocal space!!!

# Summary & Overview

## Bravais Lattices

$$\Psi_k(r) = \Psi_0 \cdot e^{i\vec{k} \cdot \vec{r}}$$

## Direct Lattice

WS fcc, WS bcc

Fourier Transform

## Reciprocal Lattice

BZ bcc, BZ fcc

$$n(x) = \sum_p n_p e^{(i2\pi p x / a)}$$

### Primitive vectors

$\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$

### Translation vector

$$\mathbf{R} = n\mathbf{a}_1 + m\mathbf{a}_2 + l\mathbf{a}_3$$

### Primitive vectors

$$\mathbf{b}_1 = 2\pi \frac{\mathbf{a}_2 \times \mathbf{a}_3}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)}; \quad \mathbf{b}_2 = 2\pi \frac{\mathbf{a}_3 \times \mathbf{a}_1}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)}; \quad \mathbf{b}_3 = 2\pi \frac{\mathbf{a}_1 \times \mathbf{a}_2}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)}$$

### Translation vector

$$\bar{\mathbf{k}} = k_1 \bar{\mathbf{b}}_1 + k_2 \bar{\mathbf{b}}_2 + k_3 \bar{\mathbf{b}}_3$$



The crystal is a periodic structure that can be represented mathematically by a Fourier Series:

$$f(x) = f_0 + \sum_{p=1}^{\infty} C_p \cos\left(\frac{2\pi p x}{a}\right) + \sum_{p=1}^{\infty} S_p \sin\left(\frac{2\pi p x}{a}\right)$$

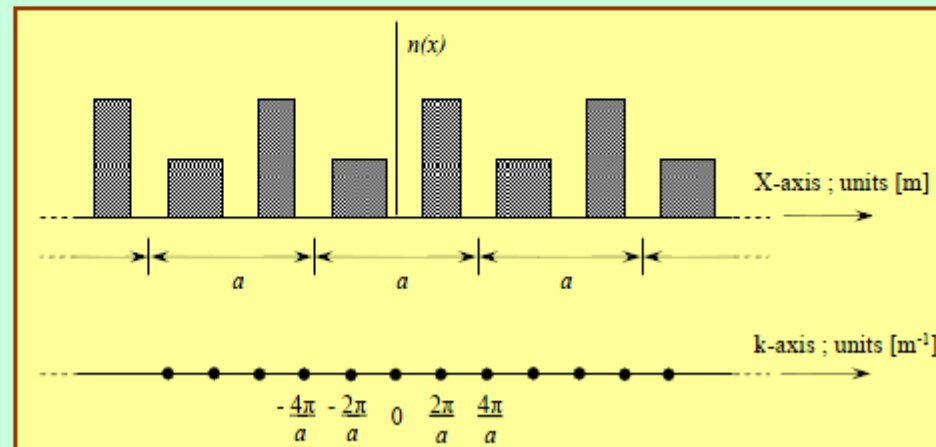
or

$$f(x) = \sum_p f_p e^{(i2\pi p x/a)}$$



For a 1D crystal the reciprocal lattice is a line of points separated by  $2\pi/a$ . The reciprocal lattice points tell us the allowed terms in the Fourier series. A term is allowed if it is consistent with the periodicity of the crystal.

A periodic function  $n(x)$  of period  $a$ , and the terms  $2\pi p/a$  that may appear in the Fourier transform of  $n(x)$



For 3D space in the case of the crystal every periodic function is associated with a [Bravais lattice](#).

You can think of the function as being defined in a primitive unit cell and then repeating the primitive unit cell at every point of the Bravais lattice. The corresponding periodic function can be written as a Fourier series in the form:

$$f(\vec{r}) = \sum_{\vec{G}} f_{\vec{G}} \exp(i\vec{G} \cdot \vec{r})$$

where the  $\vec{G}$ 's are the reciprocal lattice vectors of the Bravais lattice defined as:

$$\vec{G} = \nu_1 \vec{b}_1 + \nu_2 \vec{b}_2 + \nu_3 \vec{b}_3 \quad \nu_1, \nu_2, \nu_3 = \dots, -2, -1, 0, 1, 2, \dots$$

and  $f_{\vec{G}}$  are complex coefficients (called the structure factors).

The Fourier series can be rewritten in terms of the primitive reciprocal lattice vectors,  $\vec{b}^j$

$$f(\vec{r}) = \sum_{\vec{G}} f_{\vec{G}} \exp(i\vec{G} \cdot \vec{r}) = \sum_{v_1=-\infty}^{\infty} \sum_{v_2=-\infty}^{\infty} \sum_{v_3=-\infty}^{\infty} f_{v_1 v_2 v_3} \exp\left(i\left(v_1 \vec{b}_1 \cdot \vec{r} + v_2 \vec{b}_2 \cdot \vec{r} + v_3 \vec{b}_3 \cdot \vec{r}\right)\right)$$

An example of a real periodic function that has an orthorhombic Bravais lattice can be constructed using the reciprocal lattice vectors 100, -100, 010, 0-10, 001, 00-1.

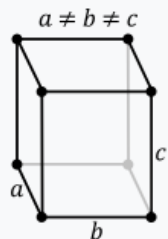
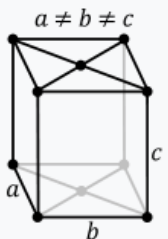
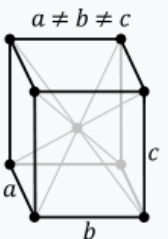
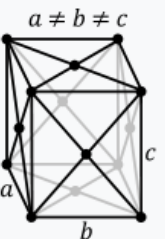
If for all of these reciprocal lattice points  $f_{\vec{G}} = 1$ , then the periodic function is:

$$\begin{aligned} f(\vec{r}) &= \exp\left(\frac{i2\pi x}{a}\right) + \exp\left(\frac{-i2\pi x}{a}\right) + \exp\left(\frac{i2\pi y}{b}\right) + \exp\left(\frac{-i2\pi y}{b}\right) + \exp\left(\frac{i2\pi z}{c}\right) + \exp\left(\frac{-i2\pi z}{c}\right) \\ &= 2\cos\left(\frac{2\pi x}{a}\right) + 2\cos\left(\frac{2\pi y}{b}\right) + 2\cos\left(\frac{2\pi z}{c}\right). \end{aligned}$$

Note1:  $e^a e^b = e^{a+b}$

Note2: Euler Relation

$$e^{ix} = \cos x + i \sin x$$

| Bravais lattice    | Primitive orthorhombic  | Base-centered orthorhombic  | Body-centered orthorhombic  | Face-centered orthorhombic  |
|--------------------|---|---|---|---|
| Pearson symbol     | oP  | oS  | oI  | oF  |
| Standard unit cell |  |  |  |  |

In a similar manner, periodic functions with a **bcc**, **fcc**, or **hexagonal** Bravais lattice can be constructed:

$$\text{bcc:} \quad f(\vec{r}) = \cos\left(\frac{\pi x}{a}\right) \cos\left(\frac{\pi y}{a}\right) + \cos\left(\frac{\pi x}{a}\right) \cos\left(\frac{\pi z}{a}\right) + \cos\left(\frac{\pi y}{a}\right) \cos\left(\frac{\pi z}{a}\right)$$

$$\text{fcc:} \quad f(\vec{r}) = \cos\left(\frac{\pi x}{a}\right) \cos\left(\frac{\pi y}{a}\right) \cos\left(\frac{\pi z}{a}\right)$$

$$\text{hexagonal:} \quad f(\vec{r}) = \cos\left(\frac{2\pi x}{a}\right) + 2 \cos\left(\frac{\sqrt{3}\pi y}{a}\right) \cos\left(\frac{\pi x}{a}\right) + \cos\left(\frac{2\pi z}{c}\right)$$

If the periodic function  $f(r)$  is known, the Fourier coefficients  $f_G$  can be determined by multiplying both sides of the previous equation(s) by  $\exp(-i\vec{G}' \cdot \vec{r})$  and integrating over a primitive unit cell:

$$\int_{\text{unit cell}} f(\vec{r}) \exp(-i\vec{G}' \cdot \vec{r}) d^3r = \sum_{\vec{G}} \int_{\text{unit cell}} f_{\vec{G}} \exp(-i\vec{G}' \cdot \vec{r}) \exp(i\vec{G} \cdot \vec{r}) d^3r$$

- The left-hand side is the Fourier transform of the function  $f(r)$  restricted to a unit cell.
- On the right-hand side, only the term where  $G = G'$  contributes and the integral evaluates to  $f_G$  times the volume  $V$  of the primitive unit cell.

$$f_{\vec{G}} = \frac{1}{V} \int f_{\text{cell}}(\vec{r}) \exp(-i\vec{G} \cdot \vec{r}) d^3r$$

- The function  $f_{\text{cell}}(r) = f(r)$  within the primitive unit cell and is zero outside the primitive unit cell.
- The Fourier coefficient  $f_G$  is the Fourier transform of the function  $f_{\text{cell}}(r)$  divided by the volume.

## Conclusion 1

The crystal due to its periodic nature can be represented by a Fourier Series

- and therefore can be Fourier transformed or converted from the xyz real space into a frequency reciprocal space! ....
- ....and therefore because we are in a frequency space our real space linear vectors are converted into periodic functions that have the form or are mathematically represented as wave functions! This is why I stated that:

The vectors in the reciprocal lattice are all the **wave vectors** which yield plane waves with the same periodicity of the Bravais lattice.

The **reciprocal lattice** is the set of all these vectors.

## Conclusion 2

Any physical property or interaction related to the crystal structure will reproduce its periodicity !

And in this sense or from this point of view the crystal will act as a Fourier Transform for these properties! And we can write:

$$F(\mathbf{s}) = \int_{\text{crystal}} \rho(\mathbf{r}) e^{-2\pi i \mathbf{r} \cdot \mathbf{s}} d\mathbf{r}.$$

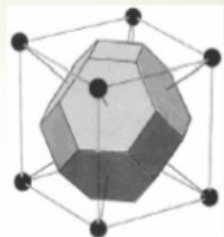
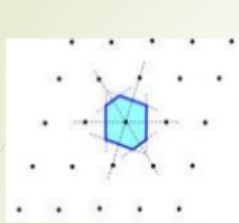
Which is the definition of Fourier Transform!

!For which the most straightforward application and visualisation of all these effects described is **XRD spectroscopy!**

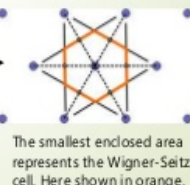
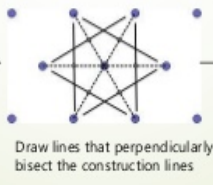
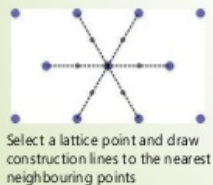
# What is the Wigner-Seitz cell? How can these cells be drawn? Do they belong to the direct space or to the reciprocal space? What is the relationship between the WZ cells and the first Brillouin zone?

- The Wigner-Seitz cell, named after Eugene Wigner and Frederick Seitz, is a primitive cell constructed by applying the **Voronoi decomposition** to a crystal lattice. It is used in the study of crystalline materials in solid-state physics.
- A Wigner-Seitz cell is an example of a primitive cell, which is a unit cell containing exactly one lattice point. For any given lattice, there are a number of possible primitive cells.

The Wigner-Seitz Cell can also be a unit cell



Wigner-Seitz cell for simple cubic in 3D



Like the Bravais lattices, they exist in both direct/real space and reciprocal space.

In reciprocal space they are the Fourier transform of one into the other and vice versa. BUT **in reciprocal space they are called Brillouin zones!**



# About the Voronoi diagrams

The partitioning of a plane with  $n$  points into convex polygons such that each polygon contains exactly one point and each point in a given polygon is closer to its creation point than to any other.

A Voronoi diagram is sometimes called a Dirichlet tessellation.

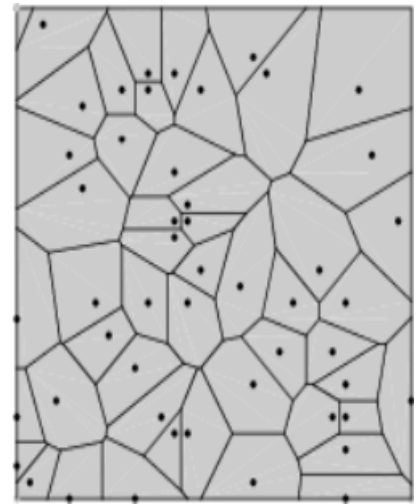
The cells are called Dirichlet regions, Thiessen polytopes or Voronoi polygons.

Voronoi diagrams were considered as early as 1644 by René Descartes and used by Dirichlet (1850) in the study of positive quadratic forms. They were also studied by Voronoi (1907), who extended the study of Voronoi diagrams to higher dimensions. They are widely used in fields such as computer graphics, epidemiology, geophysics and meteorology. One particularly notable application of a Voronoi diagram was the analysis of the 1854 cholera epidemic in London, where doctor John Snow found a strong correlation of deaths with proximity to a particular (and infected) water pump in Broad Street.

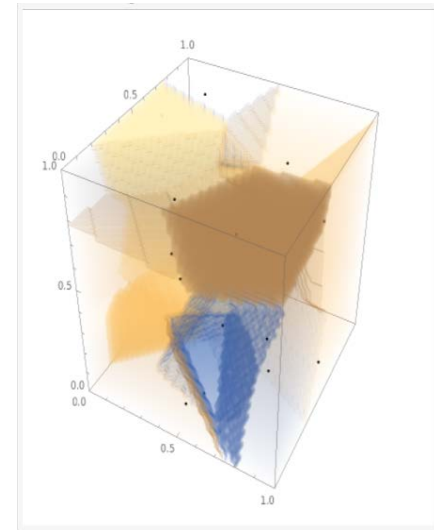
**More details can be found here:**

<https://mathworld.wolfram.com/VoronoiDiagram.html>

<https://de.wikipedia.org/wiki/Voronoi-Diagramm>



2D Voronoi  
decomposition



3D Voronoi  
decomposition

# What are Brillouin zones? How are they obtained? Why do we only consider the 1st Brillouin zone in solid state physics?

The Brillouin zone is a very important concept in solid state physics; it plays a major role in the theoretical understanding of the elementary ideas of electronic energy bands. **The first Brillouin zone is defined as the Wigner-Seitz primitive cell of the reciprocal lattice.** It is therefore the set of points in the reciprocal space that is closer to  $K = 0$  than to any other reciprocal lattice point.

The first Brillouin zone can also be defined as the set of points that can be reached from the origin without crossing a Bragg plane (except that the points lying on the Bragg planes are common to two or more zones). The second Brillouin zone is the set of points that can be reached from the first zone by crossing only one Bragg plane. Equivalently, this is the Voronoi cell around the origin of the reciprocal lattice.

To obtain the second Brillouin zone, one must first find the reciprocal lattice vectors from the lattice vectors of the real space and construct the reciprocal lattice. One of the points of the reciprocal lattice is then determined to be the origin.

There are also second, third, etc. Brillouin zones corresponding to a sequence of disjoint regions (all with the same volume) at increasing distance from the origin, but these are less commonly used. Therefore, the **first Brillouin zone is often referred to simply as the Brillouin zone.** In general, the  $n$ th Brillouin zone consists of the set of points that can be reached from the origin by crossing exactly  $n - 1$  different Bragg planes. A related concept is that of the irreducible Brillouin zone, which is the first Brillouin zone reduced by all symmetries in the point group of the lattice (point group of the crystal).

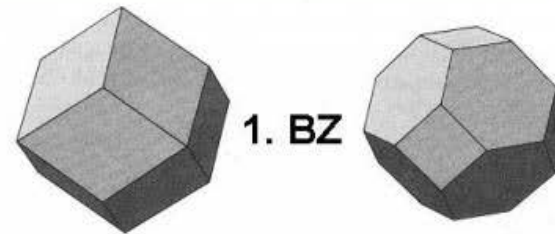
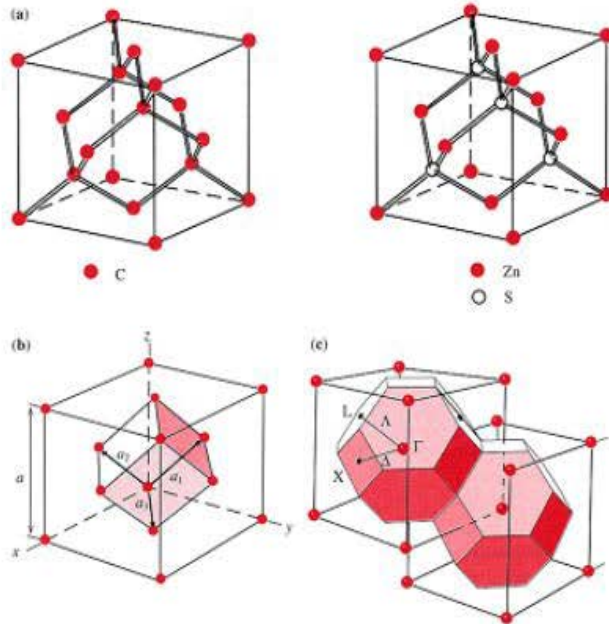
**More Informations here:**

<https://de.wikipedia.org/wiki/Brillouin-Zone>

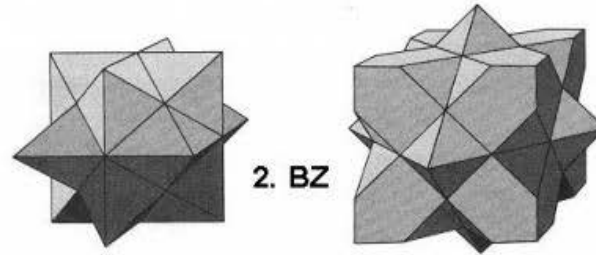
<https://www.sciencedirect.com/topics/physics-and-astronomy/brillouin-zones>

# 3D Brillouin zones

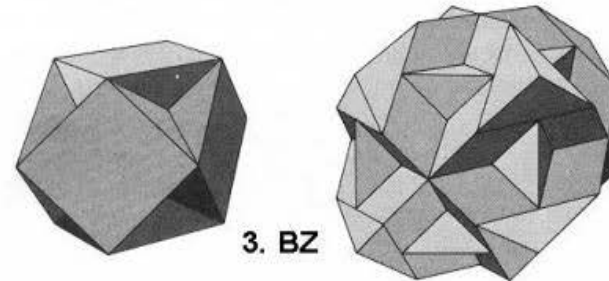
• Constructing Brillouin zones is a good example for the evolution of complex systems from the repeated application of simple rules to simple starting conditions - any **12-year old** can do it in two dimensions, but in 3D, ... Ph.D. thesis in 1965 ...



1. BZ



2. BZ

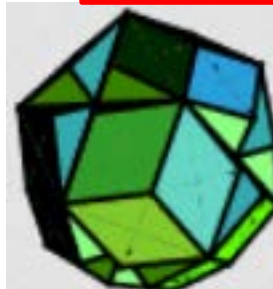


3. BZ

bcc

fcc

SC



4. BZ



4. BZ



## Next Lecture

X-Ray Diffraction basics

&

Multipurpose X-ray diffraction system  
with built-in intelligent guidance

X-Ray Diffraction basics

&

Multipurpose X-ray diffraction  
system  
with built-in intelligent guidance

with built-in intelligent guidance  
system

Multipurpose X-ray diffraction

&

YES!

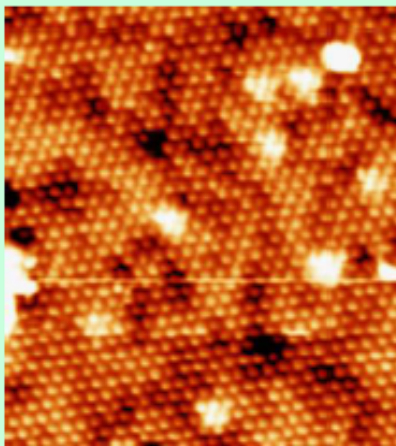
We can also see the reciprocal space and the reciprocal structures.



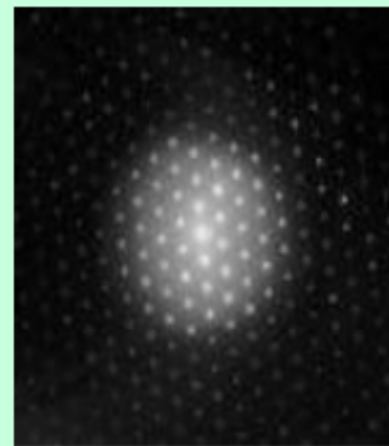
## X-Ray Diffraction: image & spectra

A diffraction pattern of a crystal is a map of the reciprocal lattice of the crystal.

A microscope image, if it could be resolved on a fine enough scale, is a map of the crystal structure in real space.



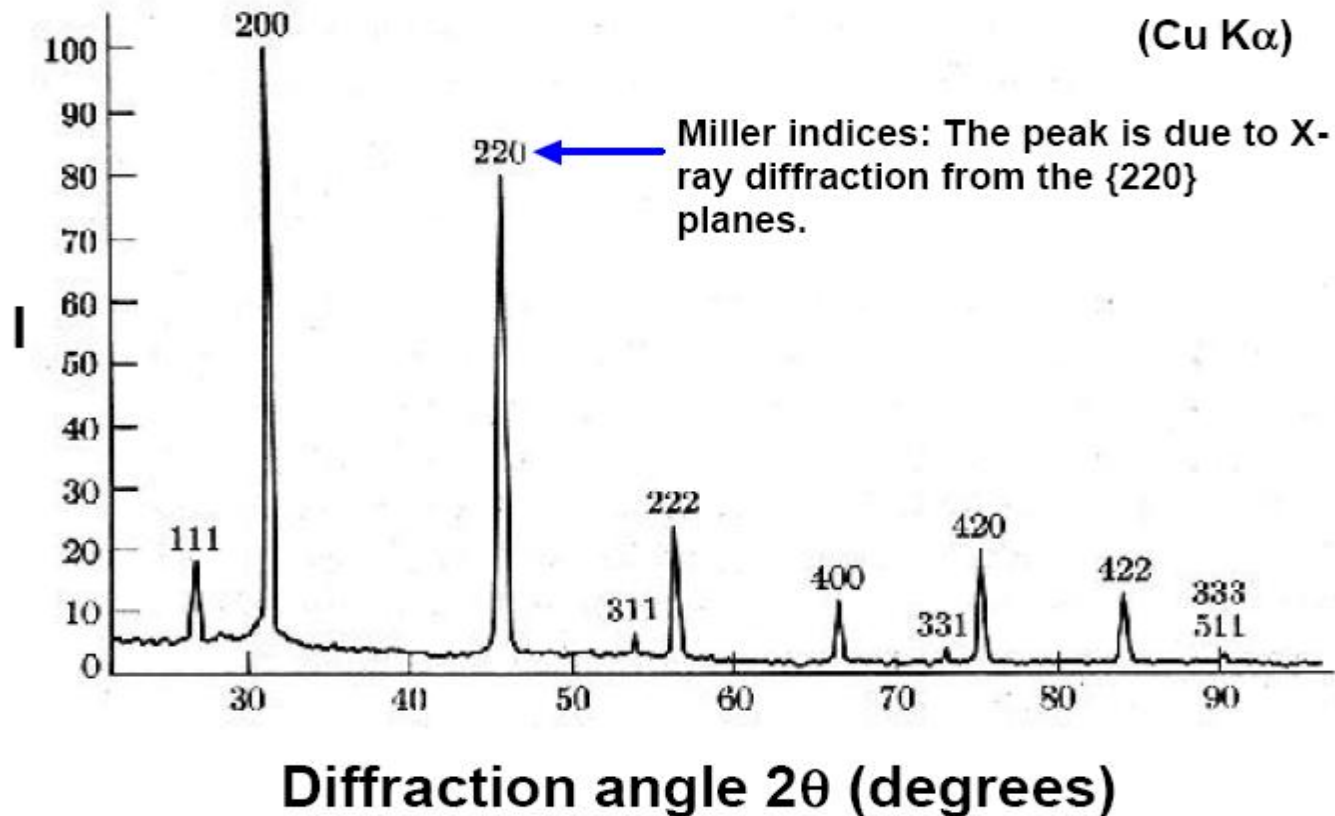
Real  
space  
image



Reciprocal  
space  
image



# XRD Pattern of NaCl Powder



Typical XRD spectra.

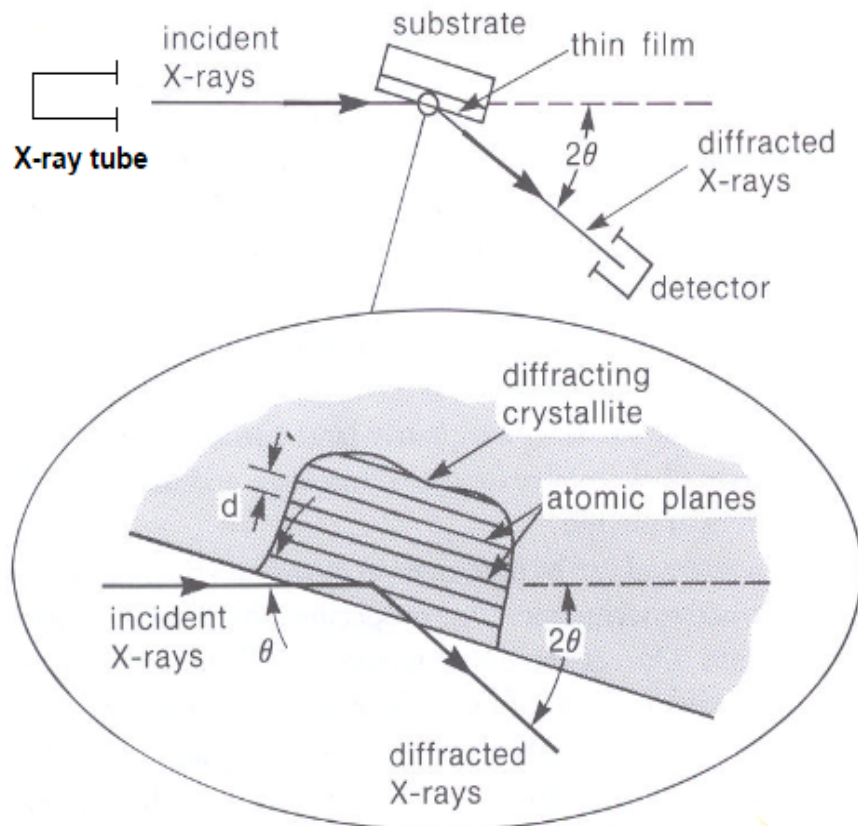
In this case NaCl has a cubic unit cell.

It is best thought of as a face-centered cubic array of anions with an interpenetrating fcc cation **lattice** (or vice-versa).

# XRD – X-ray Diffraction

## Characterization of materials Crystal Structure

### Basic Features of Typical XRD Experiment



- 1) Production
- 2) Diffraction
- 3) Detection
- 4) Interpretation

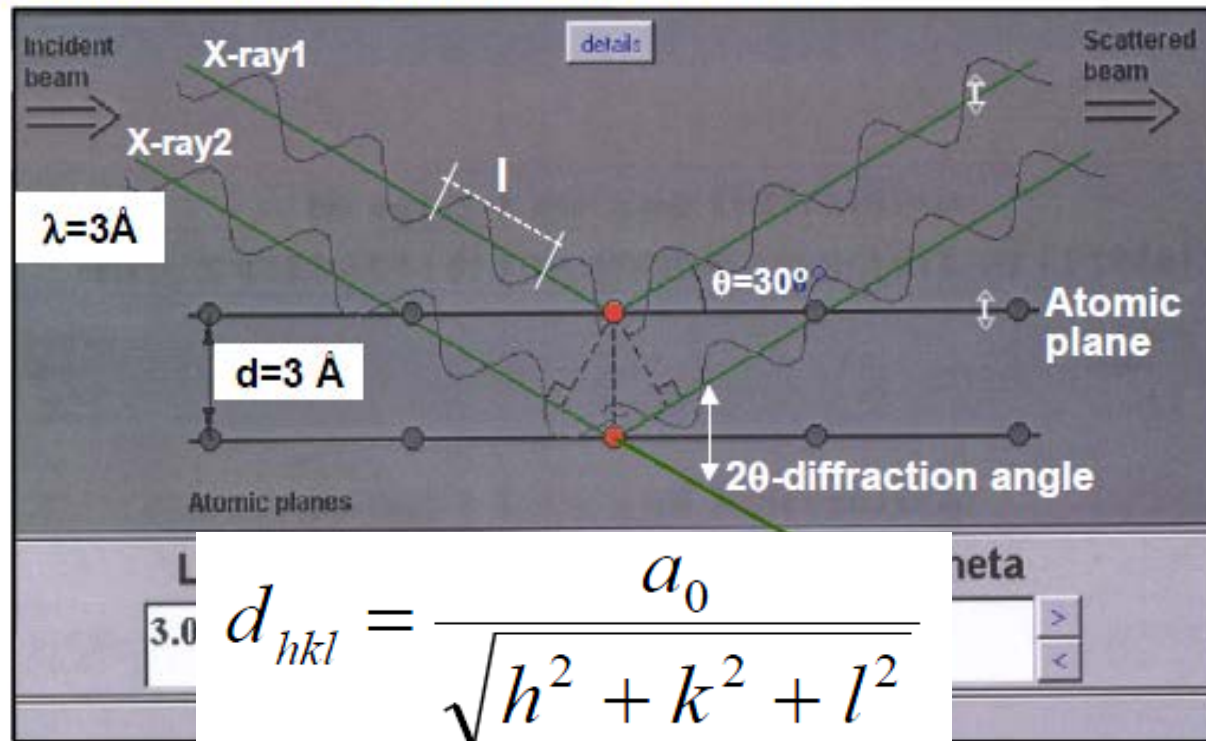


# Bragg's Law and Diffraction:

How waves reveal the atomic structure of crystals

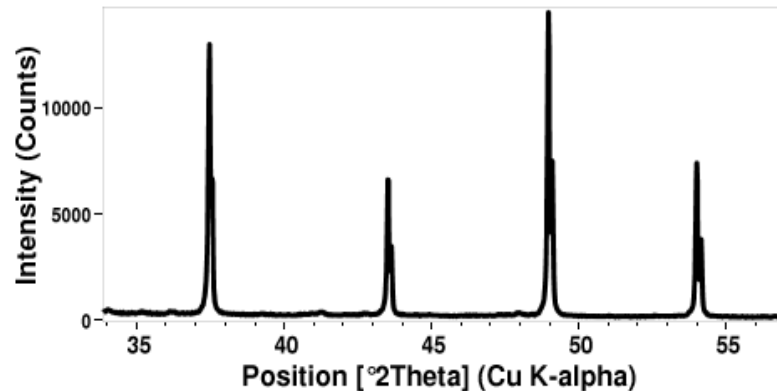
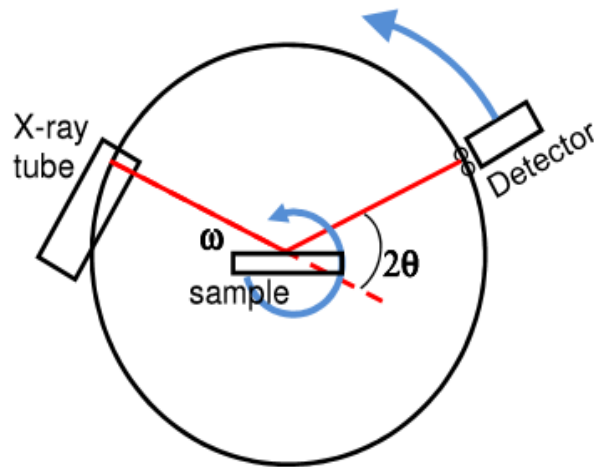
$$n \lambda = 2d_{hkl} \sin \theta_{hkl} \quad n\text{-integer}$$

Diffraction occurs only when Bragg's Law is satisfied Condition for constructive interference (X-rays 1 & 2) from planes with spacing  $d$



Different planes have different spacings  
To satisfy Bragg's law  $\Theta$  must change as  $d$  changes  
 $\Theta$  increases as  $d$  decreases and vice versa

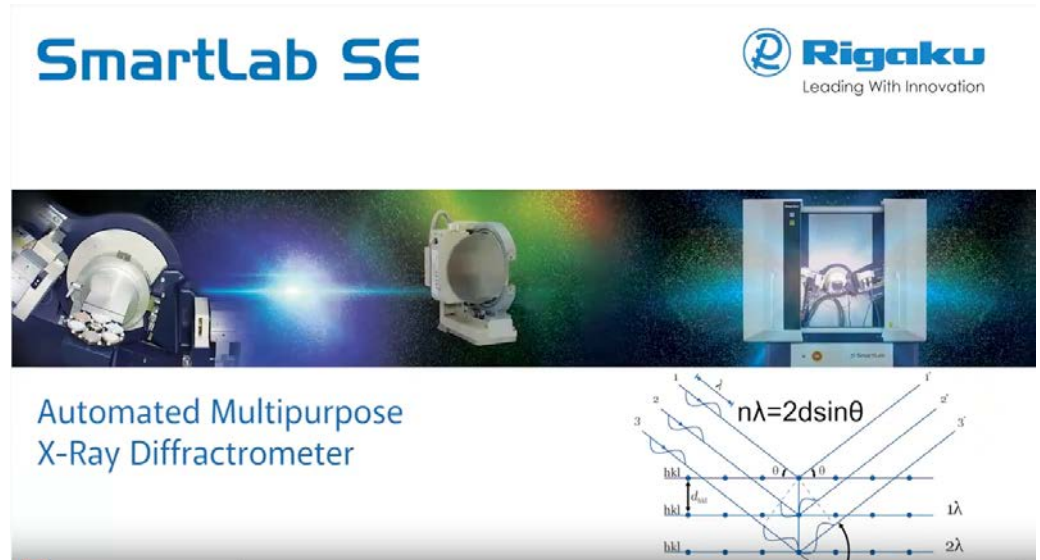
# An X-ray diffraction pattern is a plot of the intensity of X-rays scattered at different angles by a sample



- The detector moves in a circle around the sample
  - The detector position is recorded as the angle  $2\theta$
  - The detector records the number of X-rays observed at each angle  $2\theta$
  - The X-ray intensity is usually recorded as “counts” or as “counts per second”
- To keep the X-ray beam properly focused, the sample will also rotate.
  - On some instruments, the X-ray tube may rotate instead of the sample.

Modern XRD machines enable more degrees of freedom and can be used for varied purposes among which **thickness** and **roughness** of thin films and the **size of nanoparticles** in solution, are much used in semiconductor research.

Our lab has one of these machines. Please, click on the links to see how these machines look like and what can be done with them!



[Detailed movement of goniometer](#)  
[Automated Multipurpose X-Ray Diffractometer](#)