2. Basic knowledge of X-rays diffraction

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2.2 Bragg’s equation and related discussion

2.3 Diffraction Equations in Reciprocal Spaces and Ewald's sphere

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2.1 Introduction to Crystallography

- Crystals

A crystal is a solid substance in which atoms, molecules or groups of atoms are periodically and regularly arranged in three-dimensional space.

Crystals:

have a specific melting point

can produce diffraction

macroscopic homogeneity

anisotropic properties

2.1 Introduction to Crystallography

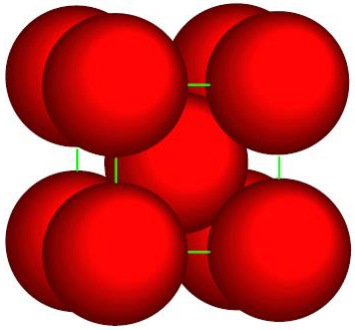
- Bravais lattice

The abstract figure in which atoms are regularly arranged in three-dimensional space in a crystal is called a spatial lattice.

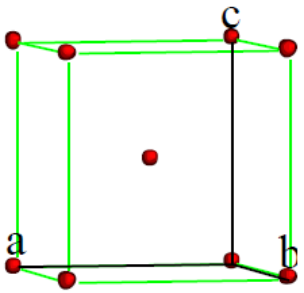
The repeating periodic vectors ***a***, ***b***, ***c*** in three directions are called basic vectors. The parallelepiped composed of basic vectors is called the unit cell.

The selection principle of the Bravais unit cell: best reflects the lattice symmetry; ***a***, ***b***, ***c*** equal as much as possible; **α**, **β**, **γ** should be right angles (90°) as much as possible.

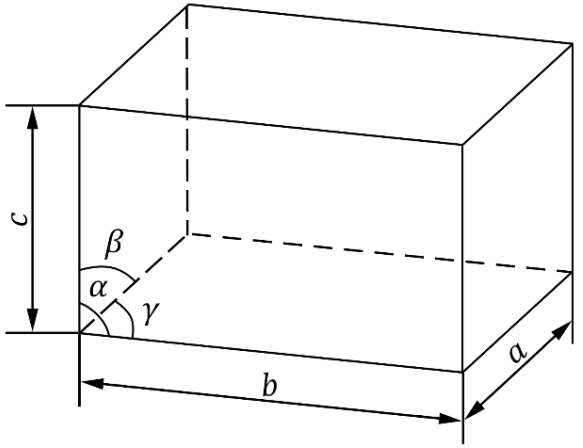
Characteristics of the Bravais unit cell: geometric relationships and calculation formulas are the simplest.



Crystal structure



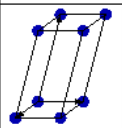
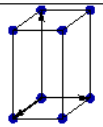
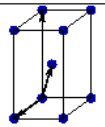
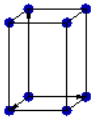
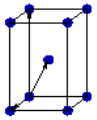
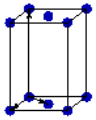
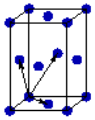
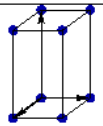
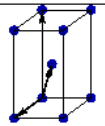
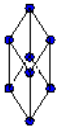
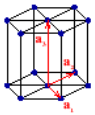
Bravais lattice



A unit cell

2.1 Introduction to Crystallography

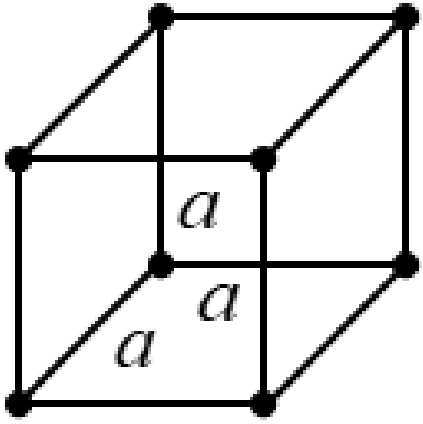
According to the symmetry of the lattice, natural crystals can be divided into **7** crystal systems. Each crystal system has up to 4 types of lattice. If there are nodes only at the corners of the unit cell, this lattice is a simple array. Sometimes there are nodes on the surface or body of the unit cell, which is called complex lattice, which includes volume centered, based centered and face centered lattice. There are only **14** Bravais lattices in the **7** major crystal systems.

Bravais lattice	Parameters	Simple (P)	Volume centered (I)	Base centered (C)	Face centered (F)
Triclinic	$a_1 \neq a_2 \neq a_3$ $\alpha_{12} \neq \alpha_{23} \neq \alpha_{31}$				
Monoclinic	$a_1 \neq a_2 \neq a_3$ $\alpha_{23} = \alpha_{31} = 90°$ $\alpha_{12} \neq 90°$				
Orthorhombic	$a_1 \neq a_2 \neq a_3$ $\alpha_{12} = \alpha_{23} = \alpha_{31} = 90°$				
Tetragonal	$a_1 = a_2 \neq a_3$ $\alpha_{12} = \alpha_{23} = \alpha_{31} = 90°$				
Trigonal	$a_1 = a_2 = a_3$ $\alpha_{12} = \alpha_{23} = \alpha_{31} < 120°$				
Cubic	$a_1 = a_2 = a_3$ $\alpha_{12} = \alpha_{23} = \alpha_{31} = 90°$				
Hexagonal	$a_1 = a_2 \neq a_3$ $\alpha_{12} = 120°$ $\alpha_{23} = \alpha_{31} = 90°$				

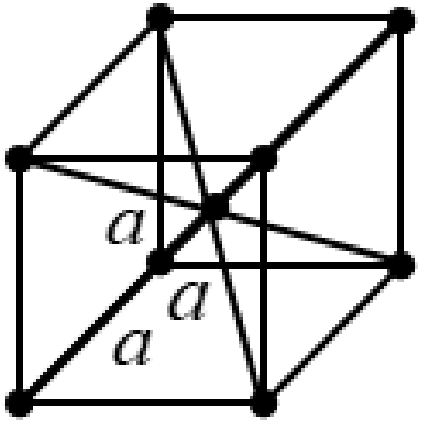
2.1 Introduction to Crystallography

- Cubic crystal system

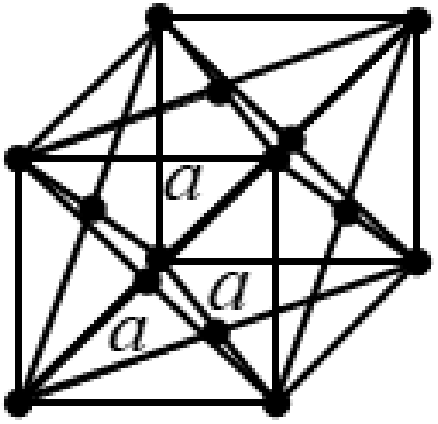
$$a = b = c, \quad \alpha = \beta = \gamma = 90°$$



Primitive cubic



Body-centered cubic

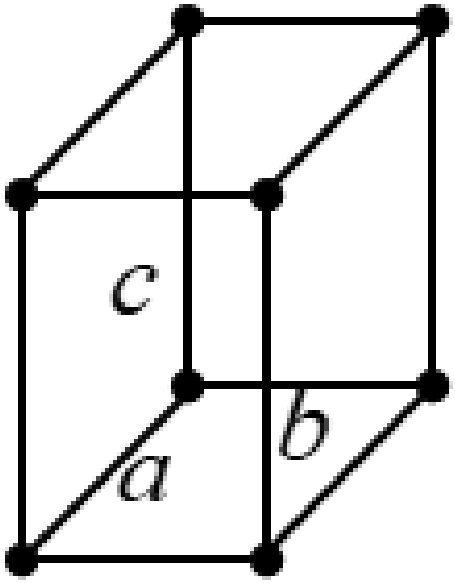


Face-centered cubic

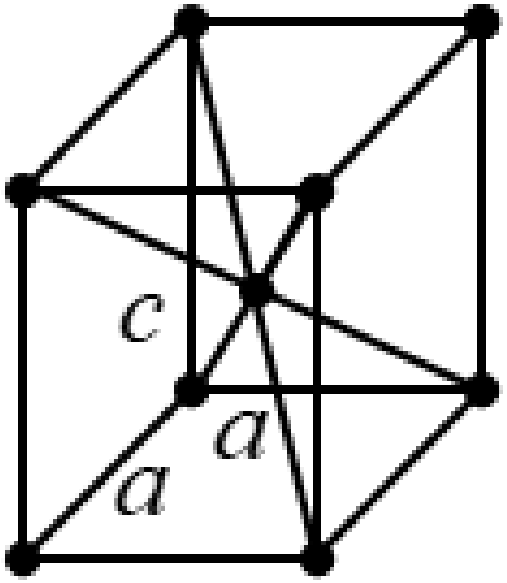
2.1 Introduction to Crystallography

- Tetragonal crystal system

$$a = b \neq c, \quad \alpha = \beta = \gamma = 90°$$



Primitive tetragonal



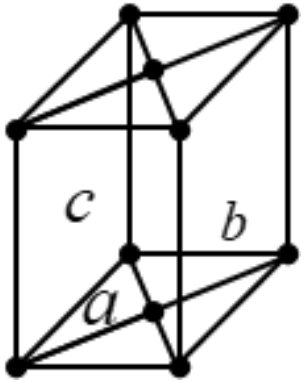
Body-centered tetragonal

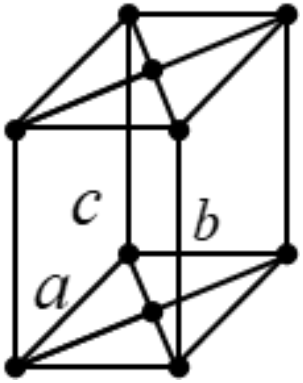
2.1 Introduction to Crystallography

- Orthorhombic crystal system

$$a \neq b \neq c, \quad \alpha = \beta = \gamma = 90°$$

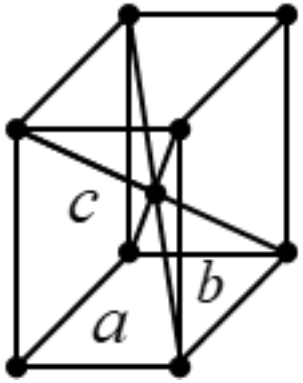
Primitive orthorhombic

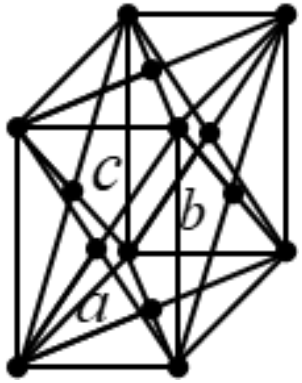




Base-centered orthorhombic

Body-centered orthorhombic



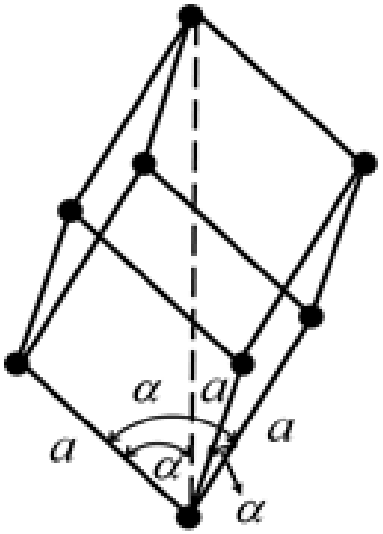


Face-centered orthorhombic

2.1 Introduction to Crystallography

- Trigonal crystal system

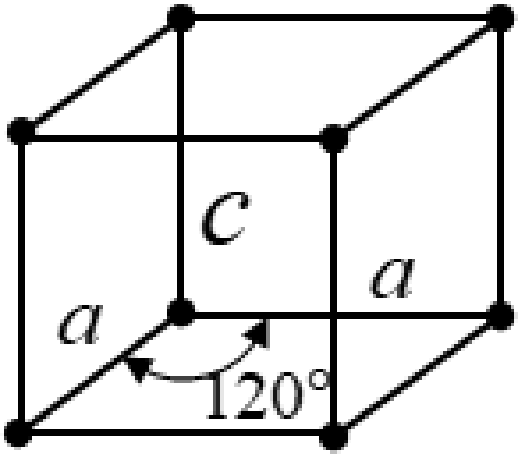
$a=b=c$，$\alpha=\beta=\gamma\neq90°$



Trigonal

- Hexagonal crystal system

$a=b\neq c$，$\alpha=\beta=90°$，$\gamma=120°$



Hexagonal

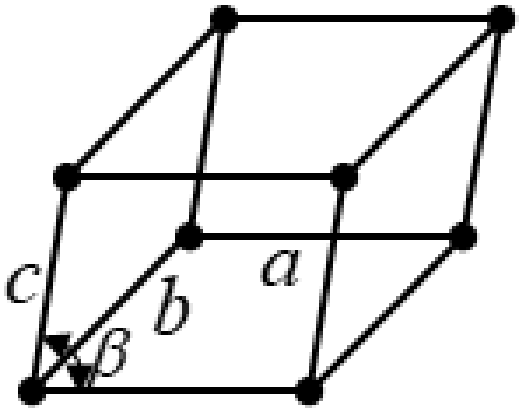
2.1 Introduction to Crystallography

- Monoclinic crystal system

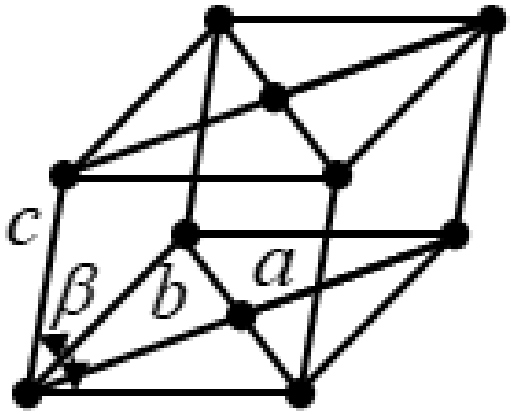
  $a \neq b \neq c$, $\alpha = \gamma = 90° \neq \beta$

- Triclinic crystal system

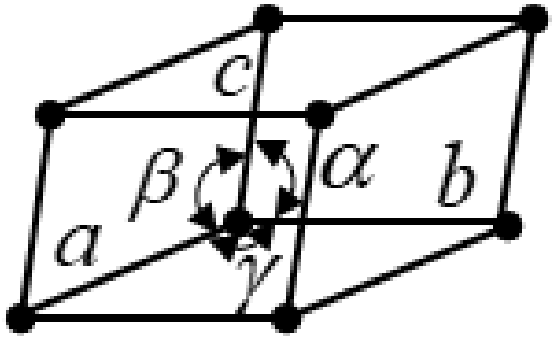
  $a \neq b \neq c$, $\alpha \neq \gamma \neq \beta \neq 90°$



Primitive monoclinic



Base-centered monoclinic



Triclinic

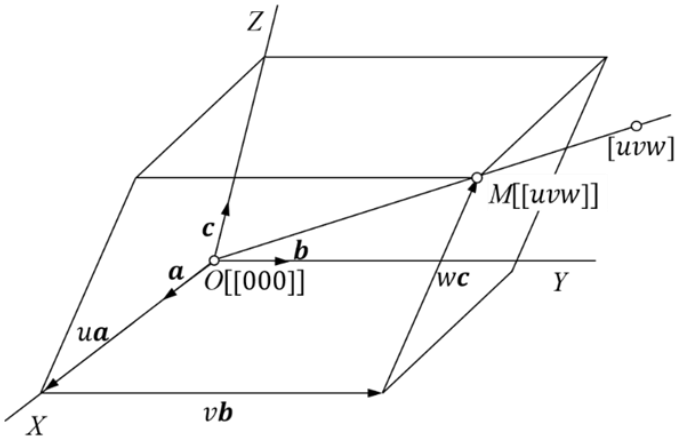
2.1 Introduction to Crystallography

- Crystallographic index

1. Crystal orientation index

The crystal lattice is composed of lattice points arranged in a certain periodic pattern in space. The crystal lattice can be decomposed into parallel straight-line clusters of nodes in any direction, and the lattice points are distributed on these straight lines. The crystal direction index [***u v w***] is used to represent a cluster of straight lines, and its determination method is shown in Figure. If the coordinates of any two points on the straight line are known to be (***X*** $_1$ ***Y*** $_1$ ***Z*** $_1$) and (***X*** $_2$ ***Y*** $_2$ ***Z*** $_2$), then ***u***, ***v***, and ***w*** are the three smallest integers.

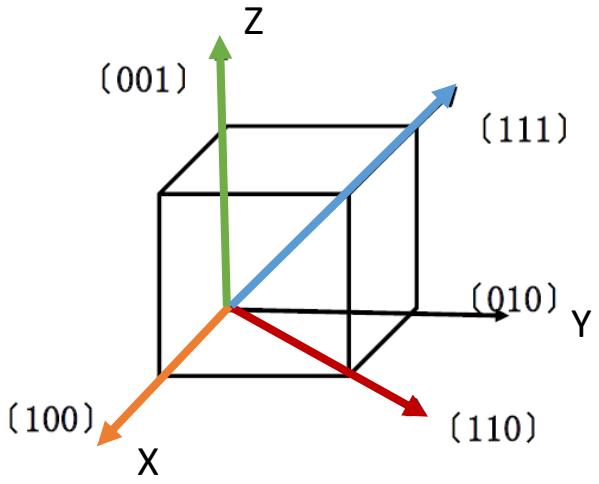
$$(X_2 - X_1):(Y_2 - Y_1):(Z_2 - Z_1) = u:v:w$$



Orientation index

[uvw]

⟨uvw⟩



2.1 Introduction to Crystallography

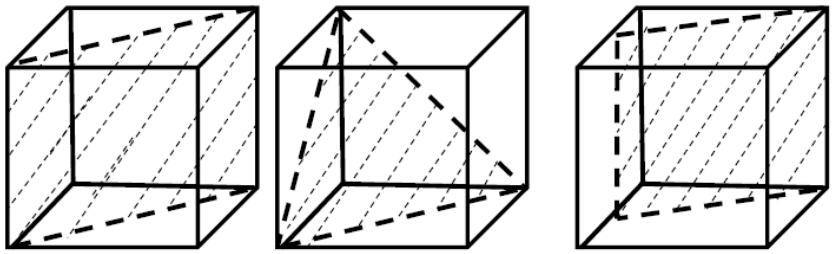
- Crystallographic index

2. Indices of crystal plane (Miller index)

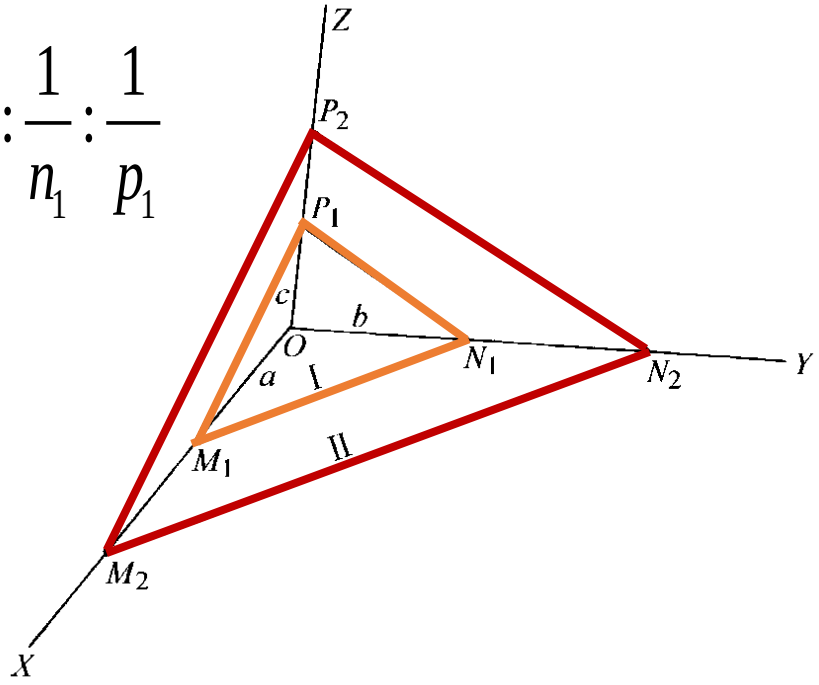
The lattice can be decomposed into arbitrarily oriented, parallel node plane clusters, Planar clusters with different orientations have different characteristics. Indicated by the facet index (***h k l***) cluster plane, ***h k l*** is its three coordinates On-axis intercept reciprocal ratio.

$$h:k:l=\frac{1}{m_2}:\frac{1}{n_2}:\frac{1}{p_2}=\frac{1}{m_1}:\frac{1}{n_1}:\frac{1}{p_1}$$

Examples:



(110) (111) (210)
{110} {111} {210}

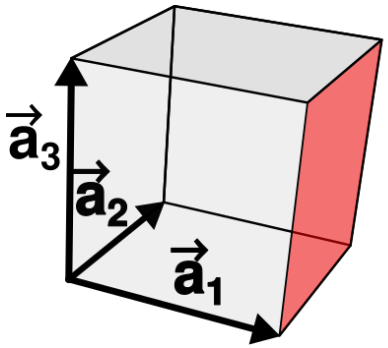


2.1 Introduction to Crystallography

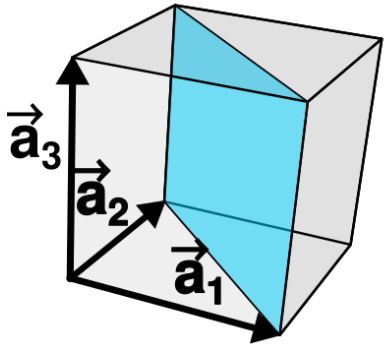
- Crystallographic index

2. Indices of crystal plane (Miller index)

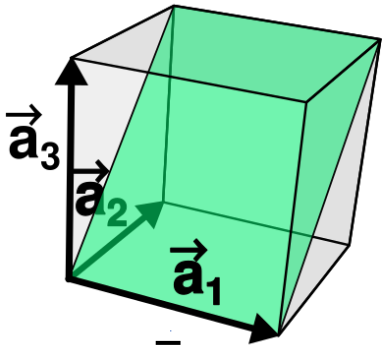
Examples



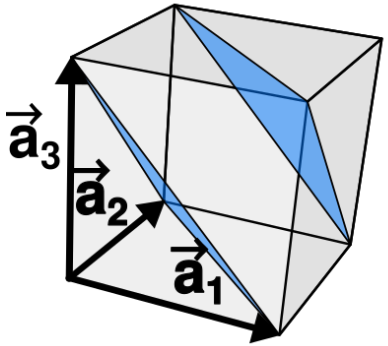
(1 0 0)



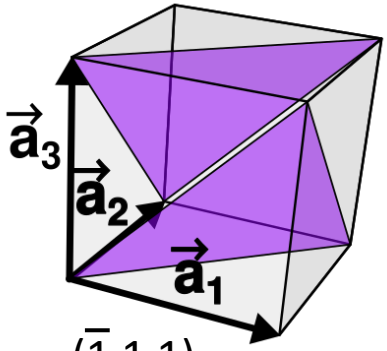
(1 1 0)



(0 $\bar{1}$ 1)



(1 1 1)

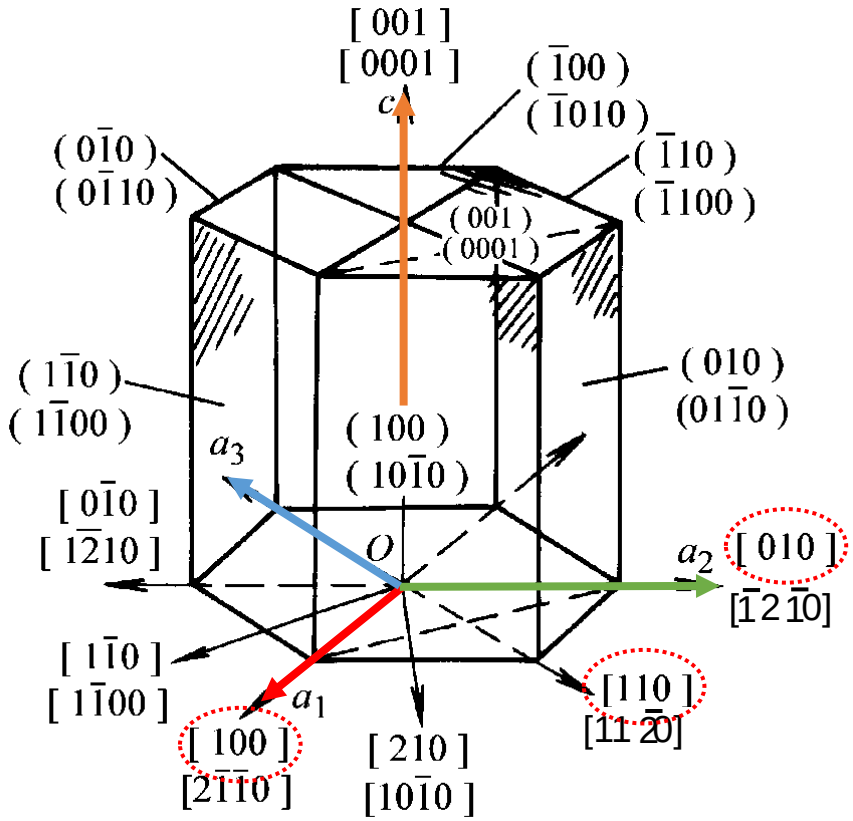


($\bar{1}$ 1 1)

2.1 Introduction to Crystallography

- Crystallographic index

3. Index of hexagonal crystal system



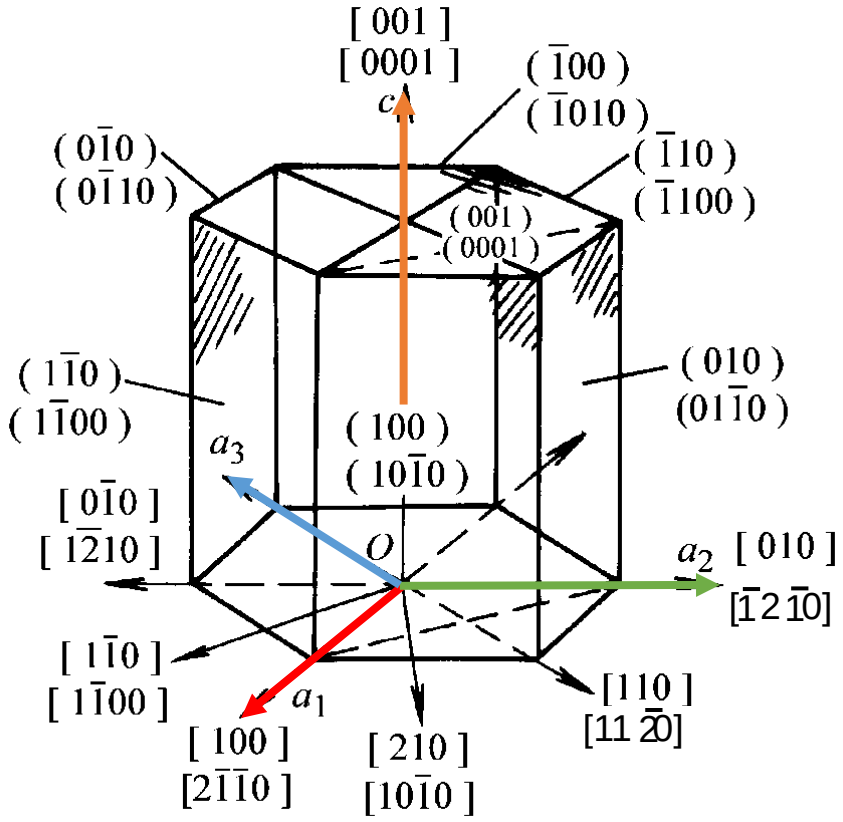
When using three indices to represent the crystal planes and directions of the hexagonal crystal system, the disadvantage is that it cannot visually display the relationship between equivalent crystal planes and equivalent crystal orientations.

e.g., (1 0 0), (0 1 0), ($\bar{1}$ 1 0) are equivalent plane.
[1 0 0], [0 1 0], [1 1 0] are equivalent direction.

2.1 Introduction to Crystallography

- Crystallographic index

3. Index of hexagonal crystal system



If the crystal plane is represented by three indices, it is (***h k l***), then the corresponding four-digit index is (***h k i l***), the top three of the four indices. Only two of the indices are independent. The relationship between them is: ***i*** = - (***h*** + ***k***)

3 indices

[1 0 0] [0 1 0] [1 1 0]

↓ ↓ ↓

[2 $\bar{1}$ $\bar{1}$ 0] [$\bar{1}$ 2 $\bar{1}$ 0] [1 1 $\bar{2}$ 0] ⟶ **⟨1 1 $\bar{2}$ 0⟩**

4 indices

3 indices

(1 0 0) (0 1 0) ($\bar{1}$ 1 0)

↓ ↓ ↓

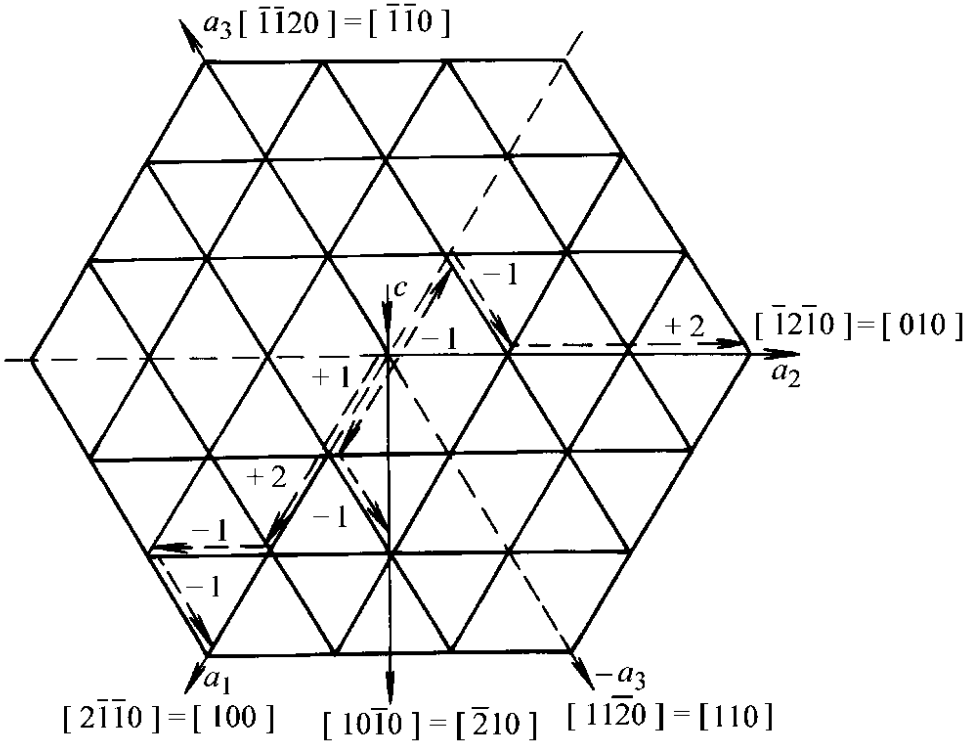
(1 0 $\bar{1}$ 0) (0 1 $\bar{1}$ 0) ($\bar{1}$ 1 0 0) ⟶ **{1 $\bar{1}$ 0 0}**

4 indices

2.1 Introduction to Crystallography

- Crystallographic index

3. Index of hexagonal crystal system



Three indices [***U V W***]

↓

Four indices [***u v t w***]

$$U = u - t,\ V = v - t,\ W = w$$

$$u = (\,2U - V\,)/3$$

$$v = (\,2V - U\,)/3$$

$$t = -\,(\,u + v\,)$$

$$w = W$$

2.1 Introduction to Crystallography

- Crystallographic index

Calculation of interplanar distance ($\boldsymbol{d}_{hkl}$)

Orthorhombic crystal system

$$d_{hkl} = \frac{1}{\sqrt{h^2/a^2 + k^2/b^2 + l^2/c^2}}$$

Tetragonal crystal system

$$d_{hkl} = \frac{1}{\sqrt{(h^2 + k^2)/a^2 + l^2/c^2}}$$

Cubic crystal system

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

Hexagonal crystal system

$$d_{hkl} = \frac{1}{\sqrt{\frac{4}{3}(h^2 + hk + k^2)/a^2 + l^2/c^2}}$$

2.2 Bragg's equation and related discussion

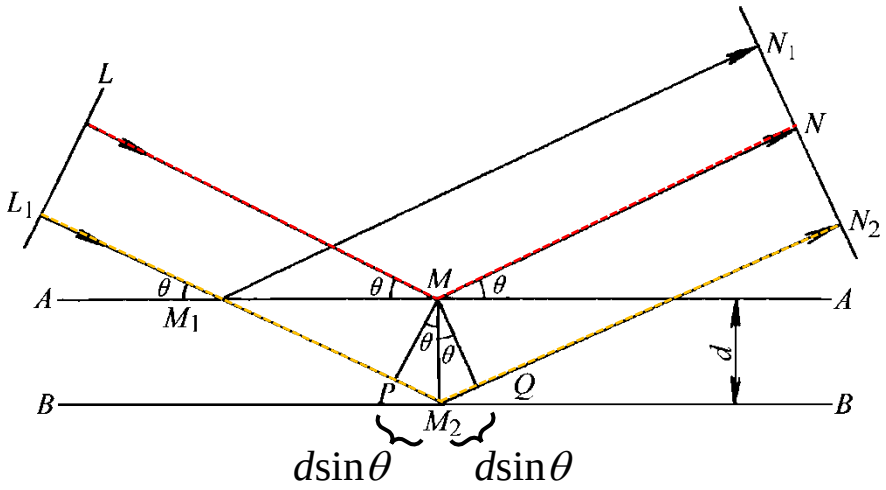
- The coherent scattered waves produced when X-rays meet tightly bound electrons in atoms strengthen each other in certain directions and weaken each other in certain directions. The total result of this scattered wave interference is called diffraction.
- Diffraction can be attributed to the two aspects: diffraction direction and diffraction intensity.
- Diffraction direction can be derived from the theory of Laue equation or Bragg's equation.
- Bragg's law regards crystal diffraction as the reflection of X-rays by crystal plane clusters in a specific direction, which is very simple and convenient.

2.2 Bragg's equation and related discussion

- Derivation of Bragg's equation

1. At LL_1, there is a beam of monochromatic parallel X-rays with the same phase (angle ϑ) When the X-ray is illuminated on the atomic plane **A-A**, it reaches NN_1 in the reflection direction, which is the same optical path;
2. The reflection line of LM that irradiates the **A-A** crystal plane is MN.
3. The incident ray L_1M_1 irradiates reflection line of adjacent crystal plane **B-B** is M_2N_2 g NN_2.

If we calculate path difference (δ) after them reaching to NN_2.

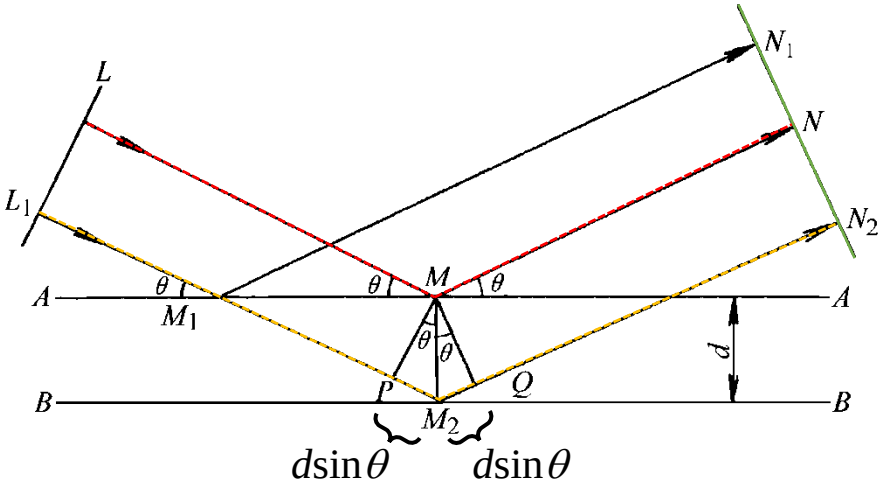


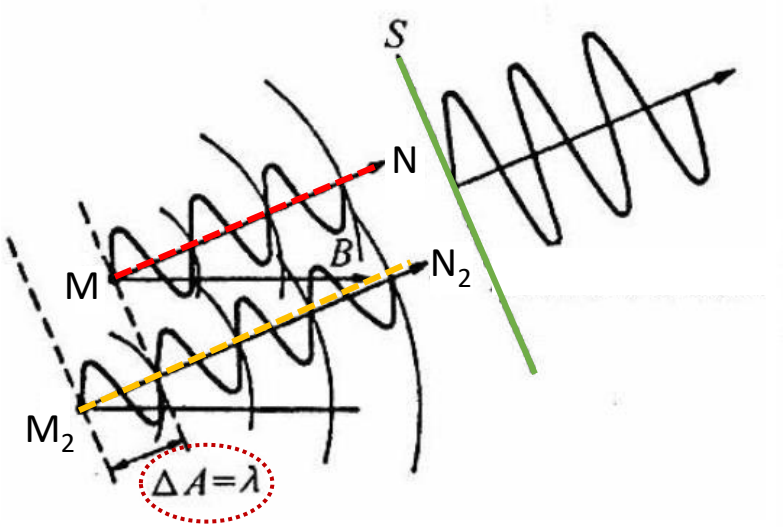
$$\delta = PM_2 + QM_2 = 2d\sin\theta$$

2.2 Bragg's equation and related discussion

- Derivation of Bragg's equation

If we calculate path difference (***δ***) after them reaching to ***NN₂***.





$$\delta = PM_2 + QM_2 = 2d\sin\theta$$

If the wavelength of X-ray is λ, then the condition of scattered waves interfere constructively should be:

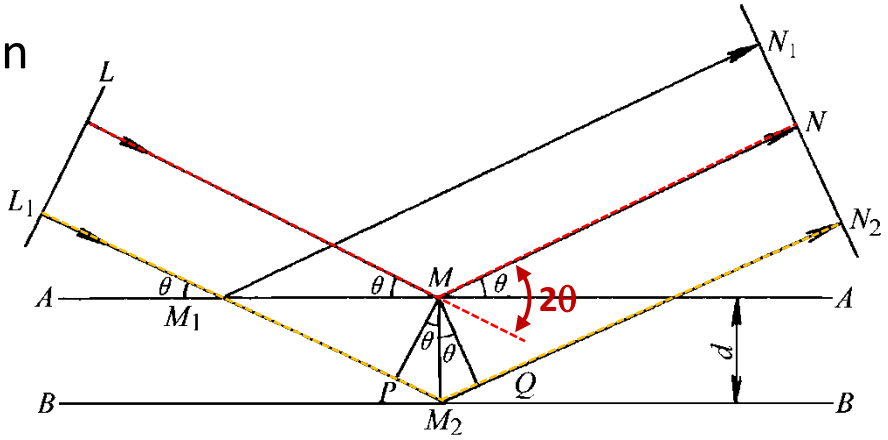
$$2d\sin\theta = n\lambda$$

This is Bragg's equation.

2.2 Bragg's equation and related discussion

- Discussion of Bragg's equation

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



1. The angle between the incident ray (or reflection ray) and the crystal plane is called the glancing angle (θ) or Bragg angle (θ); the angle between the incident ray and the diffraction ray (2θ) is called the diffraction angle; **n** is called the diffraction order.

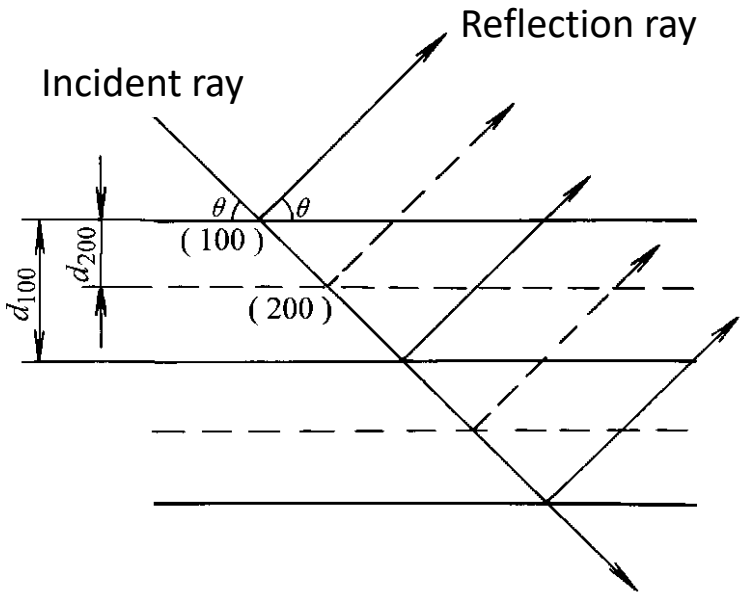
2. Treating diffraction as reflection is the basis of Bragg's equation. The crystal plane diffraction of X-rays is different from the specular reflection of light. X-rays can only be reflected in the **θ** direction that satisfies the Bragg's equation, so it is called selective reflection.

3. The Bragg's equation simply and clearly points out the necessary conditions and diffraction directions to obtain X diffraction, and gives the relationship between **d**, **θ**, **n** and **λ**.

2.2 Bragg's equation and related discussion

- Discussion of Bragg's equation

Diffraction order (**n**)



If X-rays irradiate (1 0 0) of the crystal with second order reflection, then we have:

$$2d_{100}\sin\theta = 2\lambda$$

Assume that the middle of the (1 0 0) plane is inserted with the (2 0 0) plane. Then, you can treat Second order reflections of (1 0 0) as first order reflections of (2 0 0), then we have:

$$2d_{200}\sin\theta = \lambda$$

$$\downarrow$$

$$2(d_{100}/2)\sin\theta = \lambda$$

$$2\frac{d}{n}\sin\theta = \lambda \quad \text{or} \quad 2d\sin\theta = \lambda$$

2.2 Bragg's equation and related discussion

- Discussion of Bragg's equation

Interference surface index

1. The n-order reflective surface n(***h k l***) of the crystal plane (***h k l***) is represented by the symbol (***H K L***) and is called a reflective surface or interference surface.

2. (***h k l***) is the actual crystal face in the crystal, (***H K L***) is just a virtual crystal face introduced to simplify the problem.

3. The interference surface index is called the interference index, ***H*** = ***nh***, ***K*** = ***nk***, ***L*** = ***nl***. When ***n*** = 1, the interference surface index is the crystal plane index.

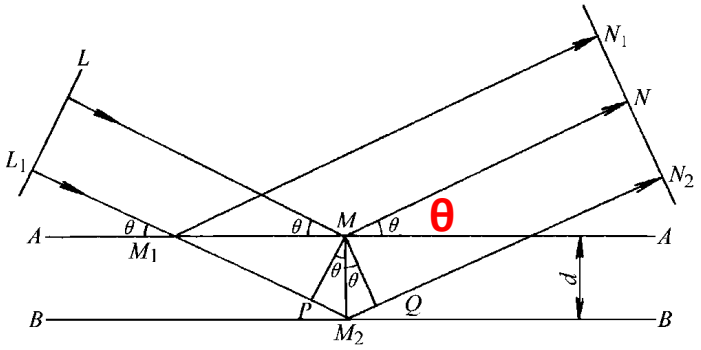
4. In X-ray structural analysis, the interplanar distance of the interference surface is generally used.

2.2 Bragg's equation and related discussion

- Discussion of Bragg's equation

Glancing angle (**θ**)

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



1. The glancing angle (**θ**) is the angle between the incident ray (or reflected ray) and the crystal plane, it is generally used to characterize the diffraction direction.

2. When ***λ*** is fixed, crystal planes with the same ***d*** must be reflected in the same direction of **θ**. When a polycrystal is irradiated with monochromatic X-rays (***λ*** is fixed), each crystal grain ***d*** has the same crystal plane, and its reflection direction (**θ**) is the same.

3. When ***λ*** is fixed, **θ** increases as the ***d*** decreases, indicating that the crystal planes with smaller spacing (***d***) correspond to larger glancing angles, otherwise the reflection lines cannot be strengthened.

2.2 Bragg's equation and related discussion

- Discussion of Bragg's equation

Diffraction conditions

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

1. The limit range of glancing angle **θ** is 0~90°, but too large or too small will cause difficulties in diffraction observation.

2. When ***d*** is constant, ***n*** increases as ***λ*** becomes smaller. Therefore, using short-wavelength X-ray irradiation, higher order reflection can be obtained.

3. Because $d\sin\theta = \lambda / 2$, so $d \geq \lambda/2$, it means that only the interference surfaces whose spacing (***d***) is greater than or equal to the half-wavelength of X-rays can participate in the reflection. When short-wavelength X-rays are used, the number of interference surfaces participating in the reflection will increase.

2.2 Bragg's equation and related discussion

- Discussion of Bragg's equation

Applications

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

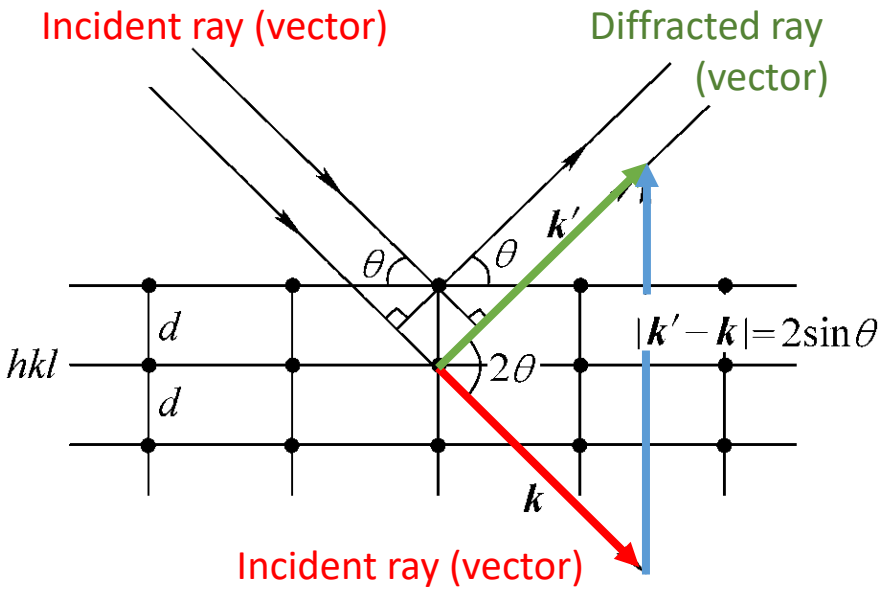
1. The Bragg's equation is the most important formula in X-ray diffraction analysis, which can explain the basic relationship of diffraction.

2. Irradiate the crystal with X-rays (known wavelength $\boldsymbol{\lambda}$) and calculate the inter-plane spacing $\boldsymbol{d}$ by measuring the diffraction angle $2\boldsymbol{\theta}$. This is X-ray structural analysis. ($\boldsymbol{\lambda}$ is know and calculate $\boldsymbol{d}$). $$\boldsymbol{d} = \frac{\lambda}{2\sin\theta}$$

3. Use a crystal (known spacing $\boldsymbol{d}$) to reflect the X-rays excited by the sample and calculate the wavelength $\boldsymbol{\lambda}$ of the X-rays through the measurement of the diffraction angle $2\boldsymbol{\theta}$. This is X-ray spectroscopic analysis. ($\boldsymbol{d}$ is know and calculate $\boldsymbol{\lambda}$) $\lambda = 2d\sin\theta$

2.3 Diffraction Equations in Reciprocal Spaces and Ewald's sphere

The difference between the unit vectors of the incident ray and the diffracted ray is perpendicular to the diffraction surface, and its absolute value is:



$$|k' - k| = 2\sin\theta$$

$$\downarrow \quad 2d\sin\theta = \lambda$$

$$|k' - k| = \frac{\lambda}{d_{hkl}}$$

$\boldsymbol{g_{hkl}}$

That is, the vector $\boldsymbol{g_{hkl}} = \boldsymbol{k'} - \boldsymbol{k}$ is perpendicular to the diffractive plane ($\boldsymbol{h\ k\ l}$). The absolute value is equal to the reciprocal of the interplanar spacing.

This result leads us to a vector space called reciprocal space.

2.3 Diffraction Equations in Reciprocal Spaces and Ewald's sphere

- The definition and properties of reciprocal lattice

The space occupied by the crystal lattice (Bravais lattice) is usually called real space. The so-called reciprocal lattice refers to another lattice corresponding to a certain real lattice in the reciprocal space (dimension is $[L]^{-1}$).

Fourier transformation

Reciprocal lattice ⟷ Real lattice

The reciprocal lattice is a crystallographic expression method established by Ewald in 1924.

The real lattice and the reciprocal lattice are the unity corresponding to each other in the real and reciprocal spaces, they are mutually reciprocal and coexist.

The reciprocal lattice reflects the periodic physical nature of the crystal lattice. It is the theoretical basis for analyzing crystal diffraction and an indispensable tool for diffraction analysis.

2.3 Diffraction Equations in Reciprocal Spaces and Ewald's sphere

- The definition and properties of reciprocal lattice

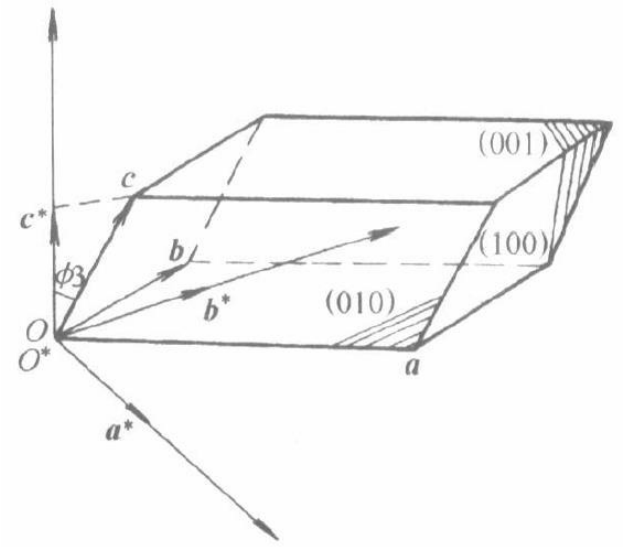
Definition of reciprocal lattice

a, ***b***, and ***c*** are unit vectors in real space, ***a****, ***b****, ***c**** are unit vectors in reciprocal space:

$$a^* = \frac{b \times c}{V}, \quad b^* = \frac{c \times a}{V}, \quad c^* = \frac{a \times b}{V}$$

V is the volume of the regular lattice unit cell.

$$V = a \cdot (b \times c) = b \cdot (c \times b) = c \cdot (a \times b)$$



$$\begin{bmatrix} \vec{a} \\ \vec{b} \\ \vec{c} \end{bmatrix} \begin{bmatrix} \vec{a}^* & \vec{b}^* & \vec{c}^* \end{bmatrix} = \begin{bmatrix} \vec{a}^* \\ \vec{b}^* \\ \vec{c}^* \end{bmatrix} \begin{bmatrix} \vec{a} & \vec{b} & \vec{c} \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} = [\mathrm{I}]$$

$$\mathrm{a}^* = \frac{\mathrm{b} \times \mathrm{c}}{\mathrm{V}}, \ \mathrm{b}^* = \frac{\mathrm{a} \times \mathrm{c}}{\mathrm{V}}, \mathrm{c}^* = \frac{\mathrm{a} \times \mathrm{b}}{\mathrm{V}}$$

$$\mathrm{V} = a \bullet (b \times c) = b \bullet (a \times c) = c \bullet (a \times b)$$

$$a^* \bullet a = b^* \bullet b = c^* \bullet c = 1$$

$$a^* \bullet b = b^* \bullet b = c^* \bullet a = 0$$

2.3 Diffraction Equations in Reciprocal Spaces and Ewald's sphere

- The definition and properties of reciprocal lattice

Properties of reciprocal lattice

1). Reciprocal lattice basic vectors

$$a^* \cdot b = a^* \cdot c = b^* \cdot a = b^* \cdot c = c^* \cdot a = c^* \cdot b = 0$$

Determine the directions of reciprocal basic vectors.

$$a^* \cdot a = b^* \cdot b = c^* \cdot c = 1$$

$$a^* = \frac{1}{a\cos(a^*, a)}, \quad b^* = \frac{1}{b\cos(b^*, b)}, \quad c^* = \frac{1}{c\cos(c^*, c)}$$

Determine the magnitudes of reciprocal basic vectors.

2.3 Diffraction Equations in Reciprocal Spaces and Ewald's sphere

- The definition and properties of reciprocal lattice

Properties of reciprocal lattice

2). Reciprocal lattice vectors

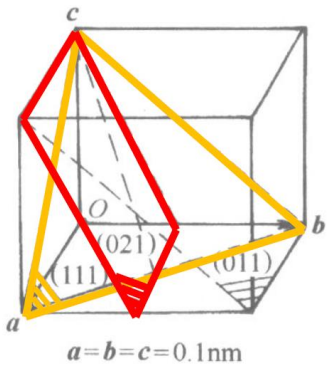
In the reciprocal space, the vector pointing from the reciprocal origin **O*** to the coordinate ***h k l*** is called reciprocal vector, denoted as $\boldsymbol{g_{hkl}}$

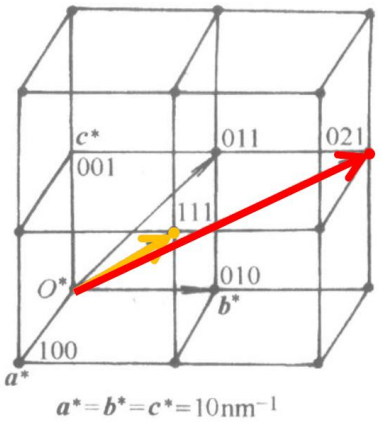
$$g_{hkl} = ha^* + kb^* + lc^*$$

The relationship between the reciprocal vector $\boldsymbol{g_{hkl}}$ and the (***h k l***) crystal plane in the real lattice is

$$g_{hkl} \perp (hkl), \quad g_{hkl} = \frac{1}{d_{hkl}}$$

Real lattice





Reciprocal lattice

$\boldsymbol{g_{hkl}}$ can be used to characterize the orientation and interplanar spacing of real lattice.

2.3 Diffraction Equations in Reciprocal Spaces and Ewald's sphere

- The definition and properties of reciprocal lattice

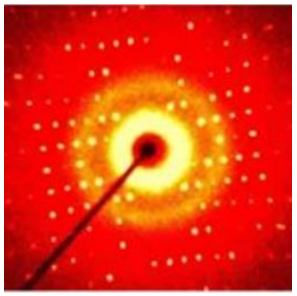
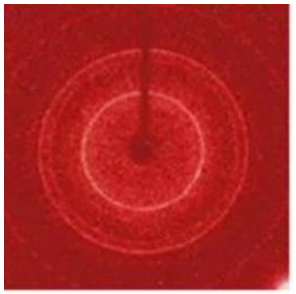
Properties of reciprocal lattice

3). Reciprocal sphere (reciprocal lattice for polycrystal)

The reciprocal lattice of a single crystal is composed of lattice points regularly arranged in a three-dimensional space. It belongs to the same crystal system as the corresponding regular lattice.

Polycrystal is composed of numerous crystal grains with different orientations, and its reciprocal lattice is composed of a series of concentric spheres with different radius.

The reciprocal vectors of the {***h k l***} crystal planes of the same family of polycrystals are arbitrarily distributed in three-dimensional space, and the reciprocal array points of their endpoints will fall on the spherical surface with O* as the center and $\mathbf{1/d}_{hkl}$ ($\boldsymbol{g}_{hkl}$) as the radius. We will discuss it later.

single crystal   Polycrystal

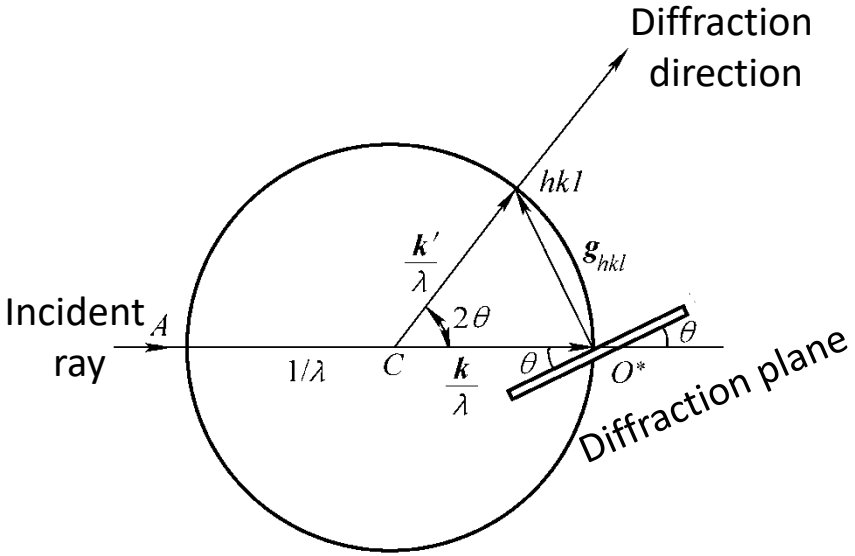
2.3 Diffraction Equations in Reciprocal Spaces and Ewald's sphere

- The Ewald's sphere

$$\frac{\boldsymbol{k}' - \boldsymbol{k}}{\lambda} = \boldsymbol{g}_{hkl}$$

This equation is the diffraction equation of reciprocal space.

1. It is easy to show that it is equivalent to Bragg's equation.
2. When diffraction occurs on the (***h k l***) plane, the λ times of its reciprocal vector $\boldsymbol{g}_{hkl}$ is equal to the difference $\boldsymbol{k}' - \boldsymbol{k}$ between the unit vectors of the incident ray and the diffracted ray.

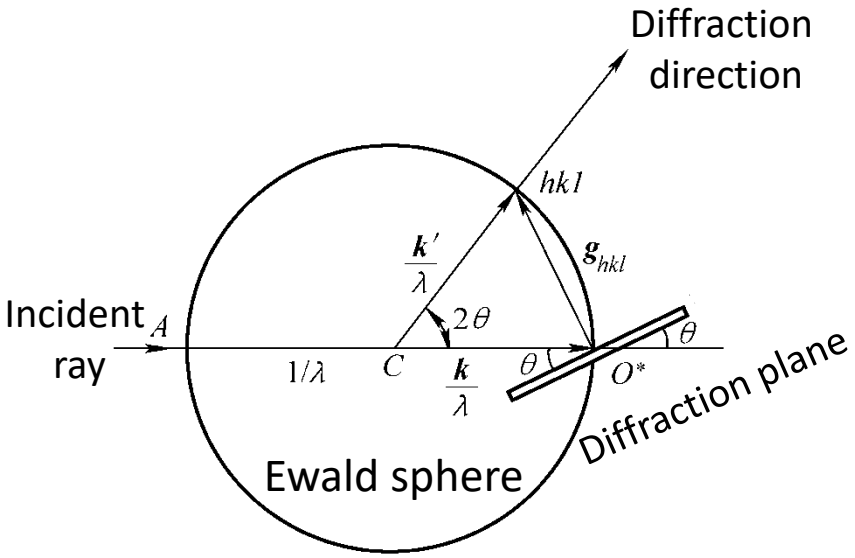


The endpoint of the incident vector points to the reciprocal origin ***O****.

Take point ***C*** in the incident direction as the center of the sphere, make a sphere with a radius of $1/\lambda$, and the sphere passes through ***O****, which is Ewald (or reflective sphere).

2.3 Diffraction Equations in Reciprocal Spaces and Ewald's sphere

- The Ewald's sphere



1. The endpoint of the incident vector points to the reciprocal origin ***O****.

2. Take point ***C*** in the incident direction as the center of the sphere, make a sphere with a radius of $1/\lambda$, and the sphere passes through ***O****, which is Ewald (or reflective sphere).

3. If a certain reciprocal point ***h k l*** is on the reflective sphere, the crystal plane will be diffracted, and the direction of the diffracted line is from the center of the reflecting sphere to the reciprocal point.

4. The Ewald diagram can illustrate whether the (***h k l***) crystal plane can diffract and the direction of the diffraction line.

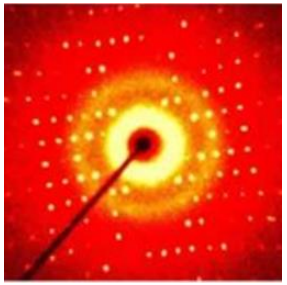
2.3 Diffraction Equations in Reciprocal Spaces and Ewald's sphere

- Characteristics of crystal diffraction patterns

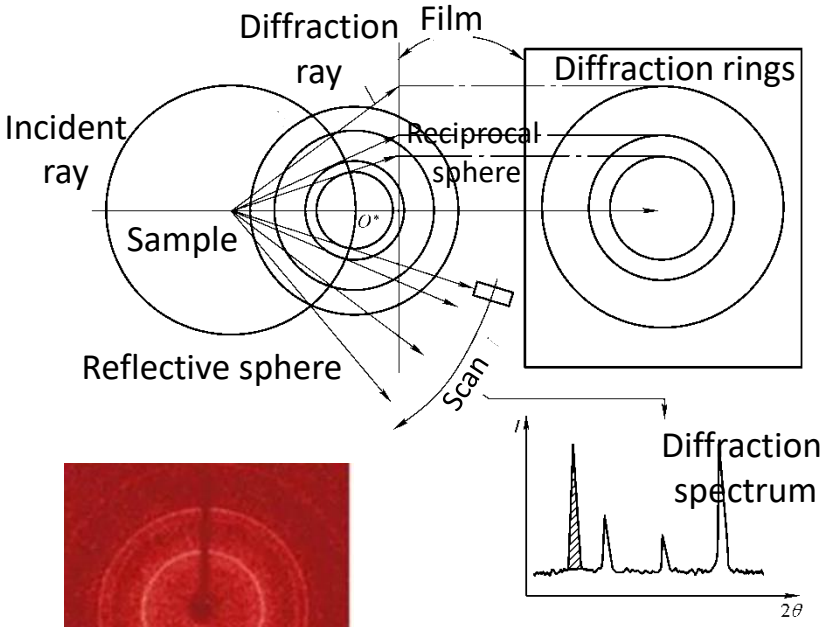
1). Single crystal diffraction pattern

Recorded with a photosensitive film placed perpendicular to the incident ray, the single crystal diffraction pattern consists of regularly arranged diffraction spots.

single crystal diffraction patterns



2). Polycrystal diffraction pattern



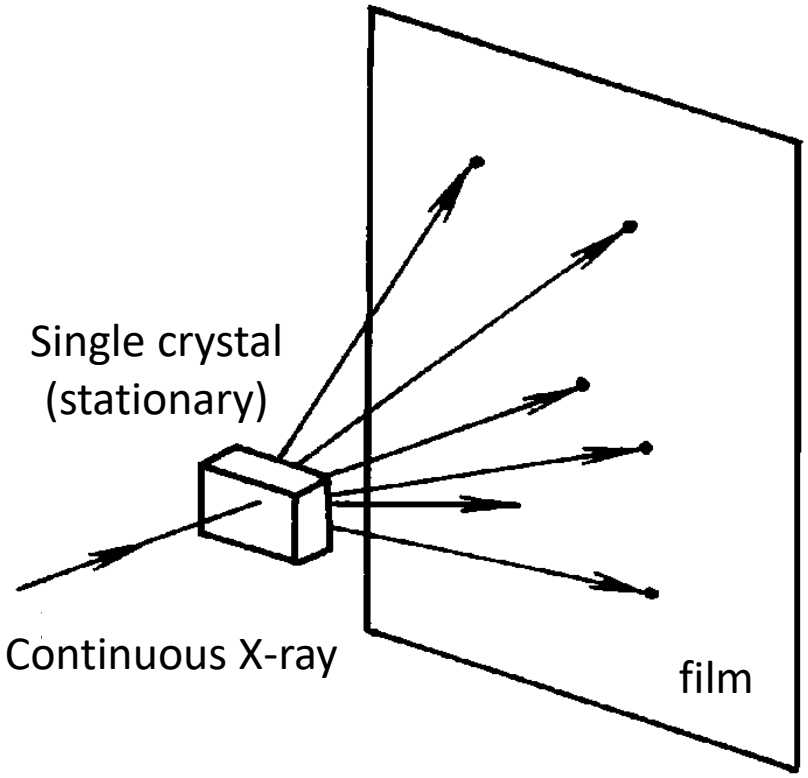
Polycrystal diffraction pattern

It is a series of concentric diffraction rings if it is recorded with a film perpendicular to the incident ray; it is a series of diffraction arcs if it is recorded with a strip film around the sample; it is a series of diffraction arcs if it is received by a counter tube scanning around the sample.

2.4 X-ray diffraction (XRD) techniques

- Laue's method

The Laue method is the earliest X-ray diffraction method. It uses continuous X-ray irradiation of a stationary single crystal and records the diffraction ray with a flat plate perpendicular to the incident ray to obtain Laue spots.



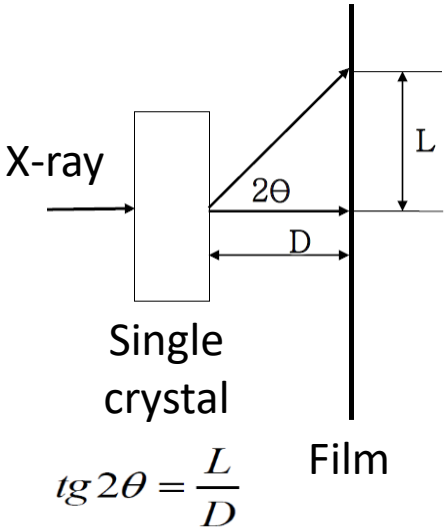
The wavelength range of the continuous spectrum is $\lambda_0 \sim \lambda_m$, only if the wavelength satisfies the Bragg's equation, the crystal plane will diffract.

Mainly used for single crystal orientation determination and crystal symmetry research.

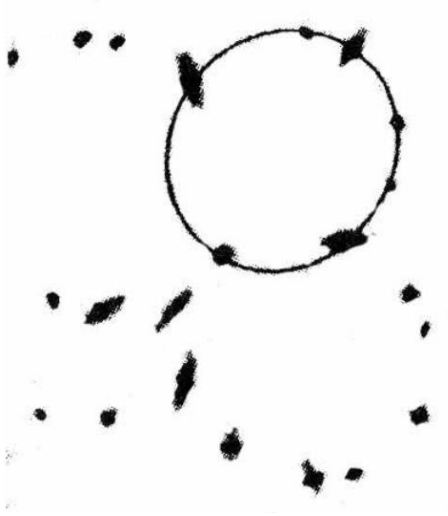
2.4 X-ray diffraction (XRD) techniques

- Laue's method

1. transmission method

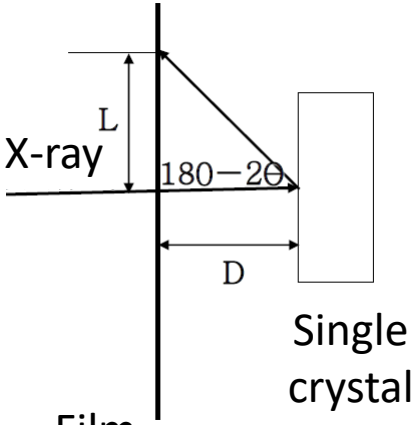


$$tg\,2\theta = \frac{L}{D}$$



Crystal plane (belongs to same crystal band)
Laue's spots are elliptical shapes

2. transmission method

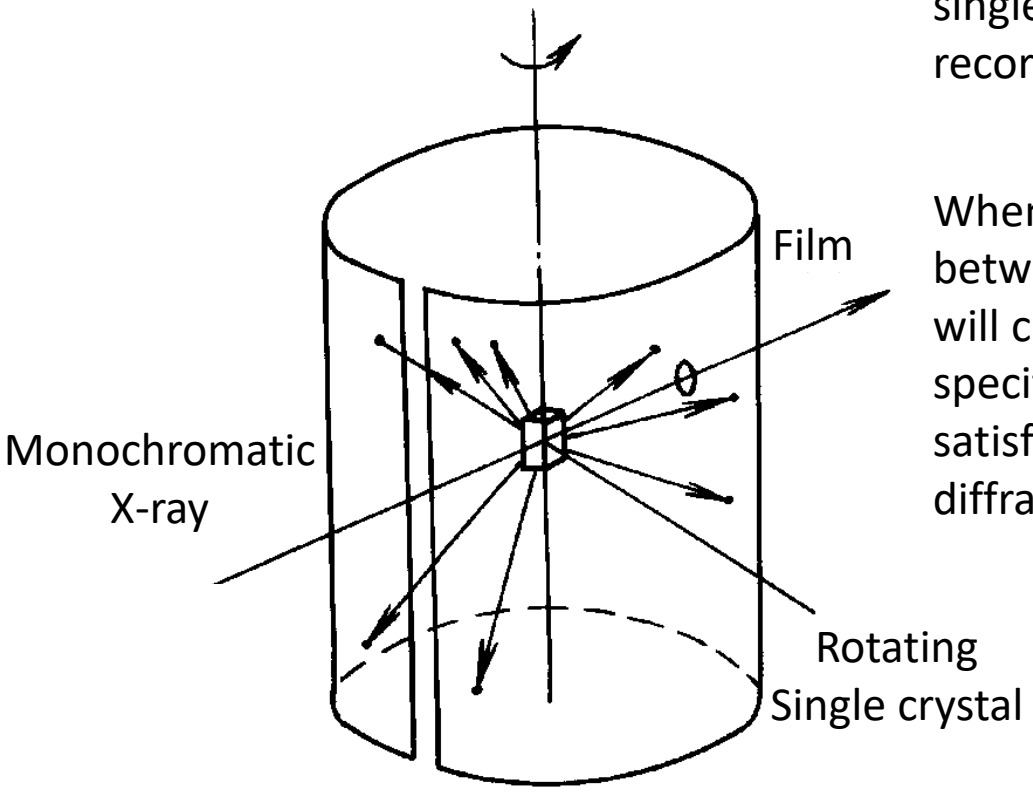


$$tg(180-2\theta) = \frac{L}{D}$$

Crystal plane (belongs to same crystal band)
Laue's spots are hyperbolic shapes

2.4 X-ray diffraction (XRD) techniques

- Rotating crystal method



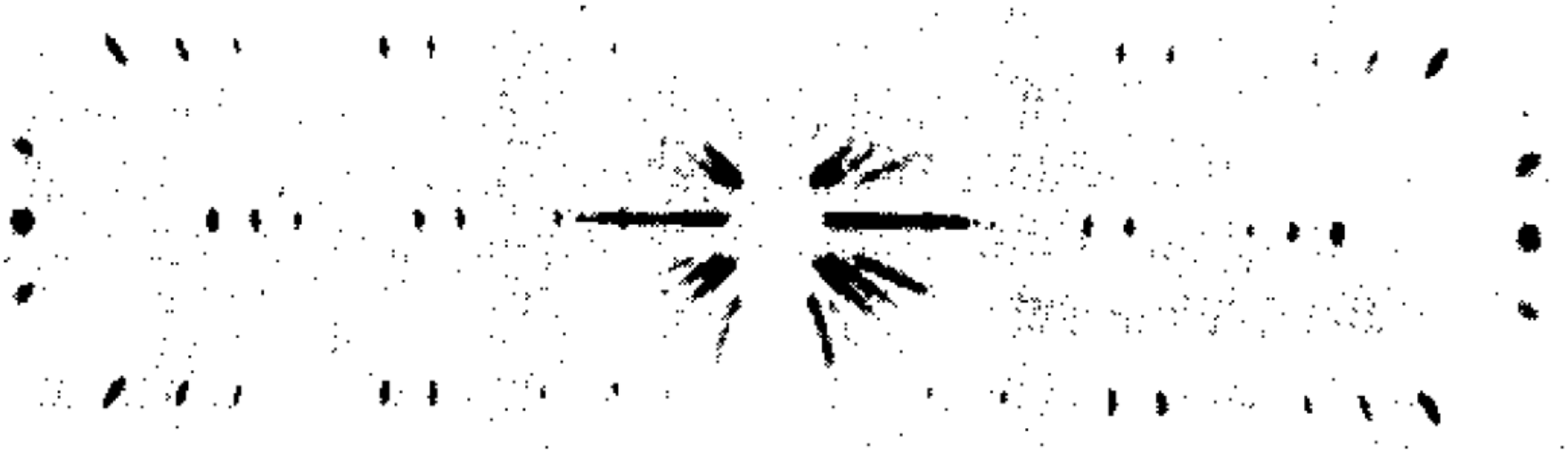
The rotating crystal method uses monochromatic X-rays to irradiate a rotating single crystal, and uses a cylindrical film to record the diffraction pattern.

When the single crystal rotates, the angle between a certain crystal plane and the X-ray will change continuously. Under some specific positions, the Bragg's conditions are satisfied, cause the film to produce diffraction spots and patterns.

Mainly used for single crystal orientation determination and crystal symmetry research.

2.4 X-ray diffraction (XRD) techniques

- Rotating crystal method

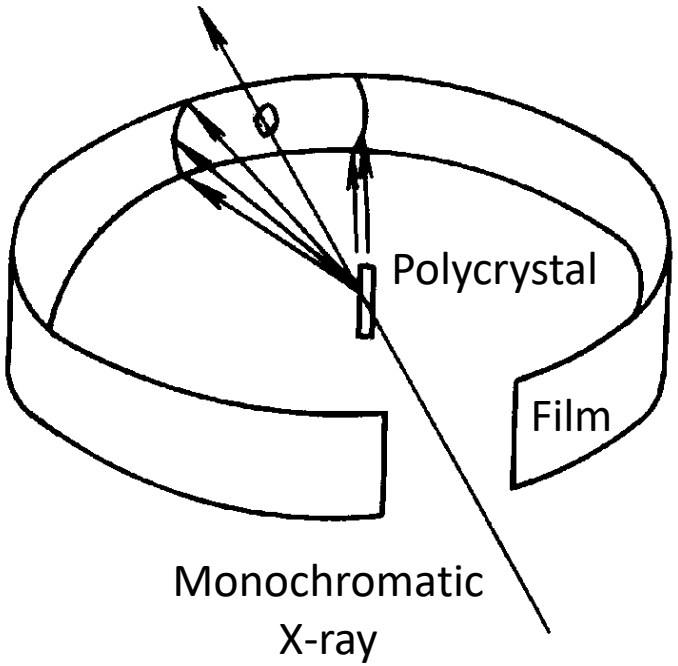


Diffraction pattern (rotating crystal method)
Sodium chloride single crystal

2.4 X-ray diffraction (XRD) techniques

- Powder method

It is the most commonly used method in diffraction analysis, and can use powder samples or block samples. Its diffraction pattern can provide a variety of information.



It can be used for crystal structure determination, qualitative and quantitative analysis of physical phases, accurate determination of lattice parameters, and determination of material internal stress, texture, grain size, etc.

Powder method is a general term for various polycrystalline X-ray analysis, The most practical method at present is the X-ray diffractometer.

2.4 X-ray diffraction (XRD) techniques

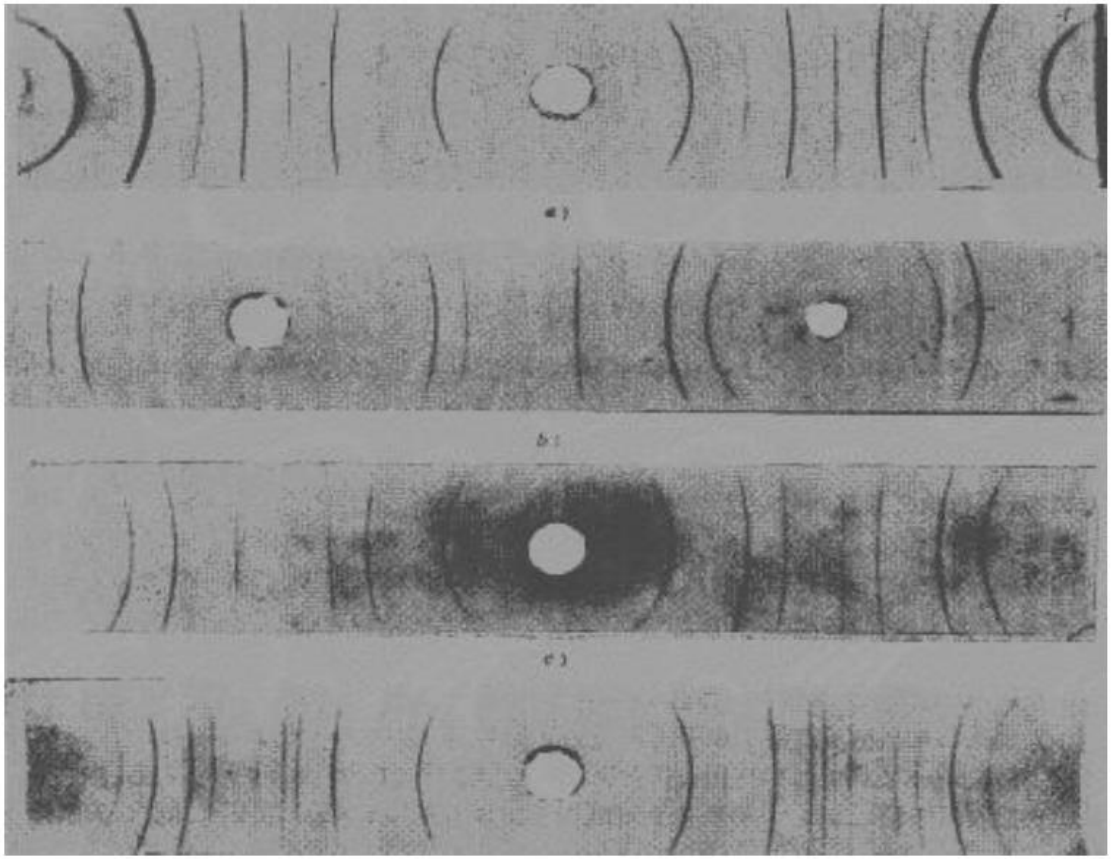
- Powder method

(a)

(b)

(c)

(d)



Body-centered cubic (tungsten)

Face-centered cubic (cobalt)

Trigonal (Silicon)

Hexagonal (zinc)