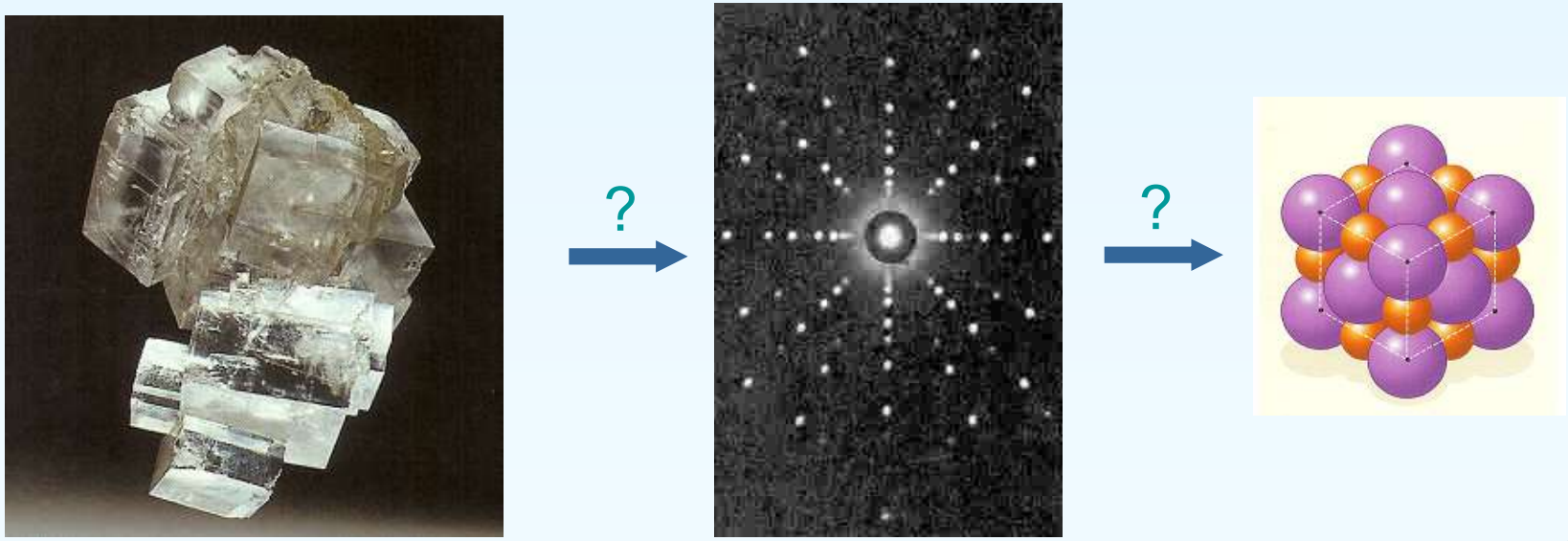
北京航空航天大學
BEIHANG UNIVERSITY

Chapter 2 Crystal Diffraction

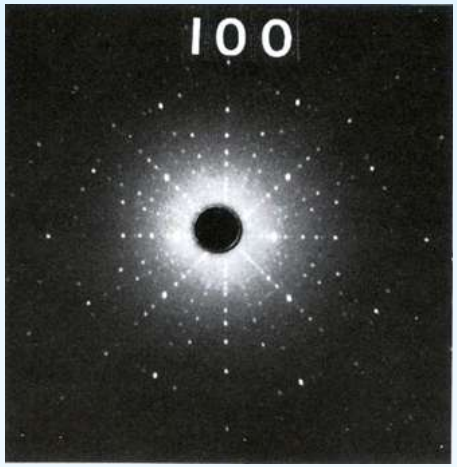
2.1 The Reciprocal Lattice

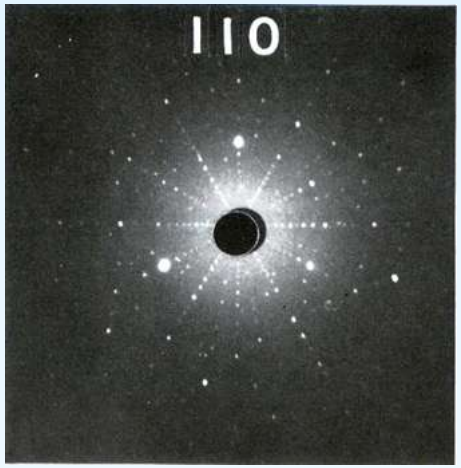
2.2 Experimental Determinations of Lattice Structures

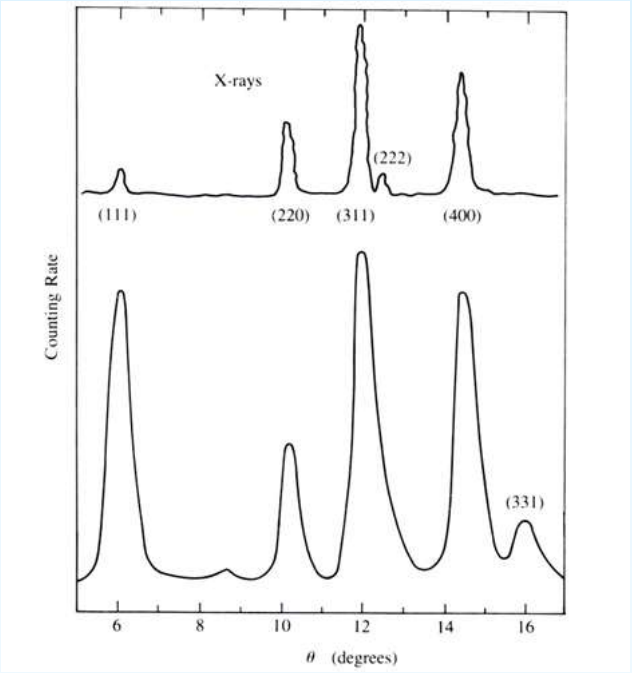


2.1 Reciprocal Lattice

How to "see" the lattice structure?







diffraction spot ↔ a family of lattice planes

reciprocal lattice ↔ direct lattice

distribution of spots → lattice structure

2.1 Reciprocal Lattice

Reciprocal lattice

2016年3月7日 22:44

Reciprocal lattice plays a fundamental role in solid state physics (periodic lattice structure)

① theory of crystal diffraction
② study of functions with the periodicity of Bravais lattice.
③ "law of momentum conservation" in discrete lattice

Consider a plane wave $e^{i\vec{k}\cdot\vec{r}}$

↳ The set of all wave vectors $\{\vec{k}\}$ that yield plane wave with the same periodicity of a given Bravais lattice $\{\vec{R}\}$ is its reciprocal lattice.

$$\Rightarrow \quad e^{i\vec{k}\cdot(\vec{r}+\vec{R})} = e^{i\vec{k}\cdot\vec{r}} \qquad \text{[same periodicity as direct lattice]}$$

$$\Rightarrow \quad e^{i\vec{k}\cdot\vec{R}} = 1$$

2.1 Reciprocal Lattice

1. Reciprocal lattice of a Bravais lattice is also a Bravais lattice

Bravais lattice: A set of discrete vectors (not all in a plane) closed by vector addition and subtraction.

Proof: $\{\vec{K}\}$ form a Bravais lattice (suppose $\{\vec{R}\}$ constitute a Bravais lattice)

$$\begin{cases} e^{i\vec{K}_1\cdot\vec{R}} = 1 \\ e^{i\vec{K}_2\cdot\vec{R}} = 1 \end{cases} \Rightarrow e^{i(\vec{K}_1+\vec{K}_2)\cdot\vec{R}} = 1 \Rightarrow \vec{K}_1 \pm \vec{K}_2 \in \{\vec{K}\}$$

2. The reciprocal of the reciprocal lattice is just the direct lattice

$e^{i\vec{G}\cdot\vec{K}} = 1, \{\vec{G}\}$ constitute nothing but the direct Bravais lattice

I. Reciprocal Lattice Vectors

Primitive vectors of a Bravais lattice: $\vec{a}_1, \vec{a}_2, \vec{a}_3$

$\vec{R}_l = l_1\vec{a}_1 + l_2\vec{a}_2 + l_3\vec{a}_3$ **generates the direct lattice**

$\vec{b}_1, \vec{b}_2, \vec{b}_3$ **are a set of vectors satisfying**

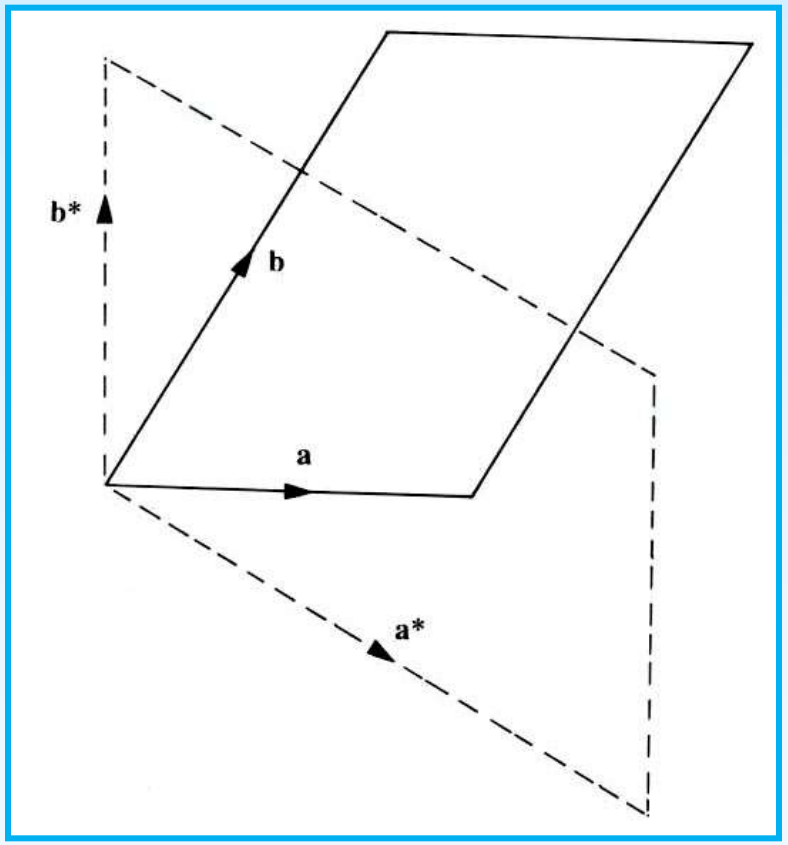
$$\vec{a}_i \cdot \vec{b}_j = 2\pi\delta_{ij} = \begin{cases} 2\pi, i = j \\ 0, i \neq j \end{cases} \qquad i, j = 1,2,3$$

$\vec{G}_h = h_1\vec{b}_1 + h_2\vec{b}_2 + h_3\vec{b}_3$ （h_1, h_2, h_3 **are arbitrary integers**）

generate the reciprocal lattice.

2.1 Reciprocal Lattice

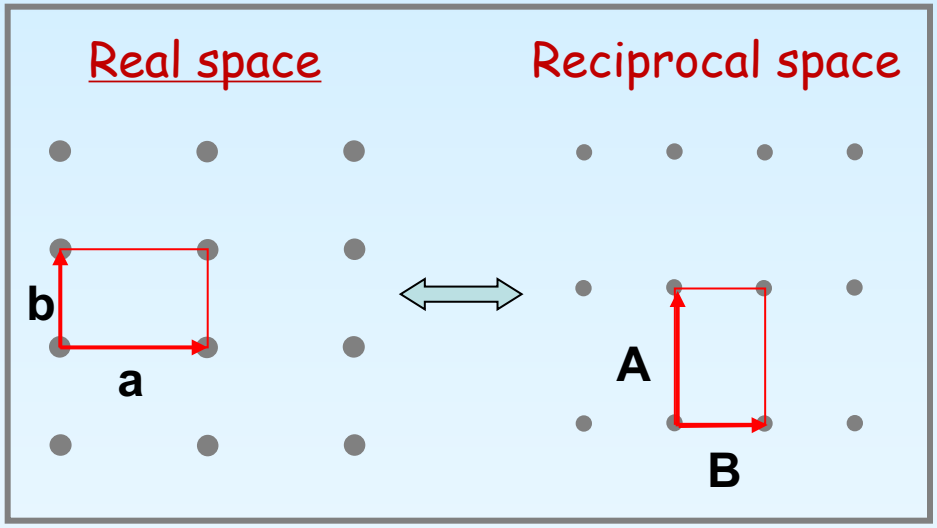
$$\begin{cases} \vec{b}_1 = 2\pi \dfrac{\vec{a}_2 \times \vec{a}_3}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)} \\ \vec{b}_2 = 2\pi \dfrac{\vec{a}_3 \times \vec{a}_1}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)} \\ \vec{b}_3 = 2\pi \dfrac{\vec{a}_1 \times \vec{a}_2}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)} \end{cases}$$

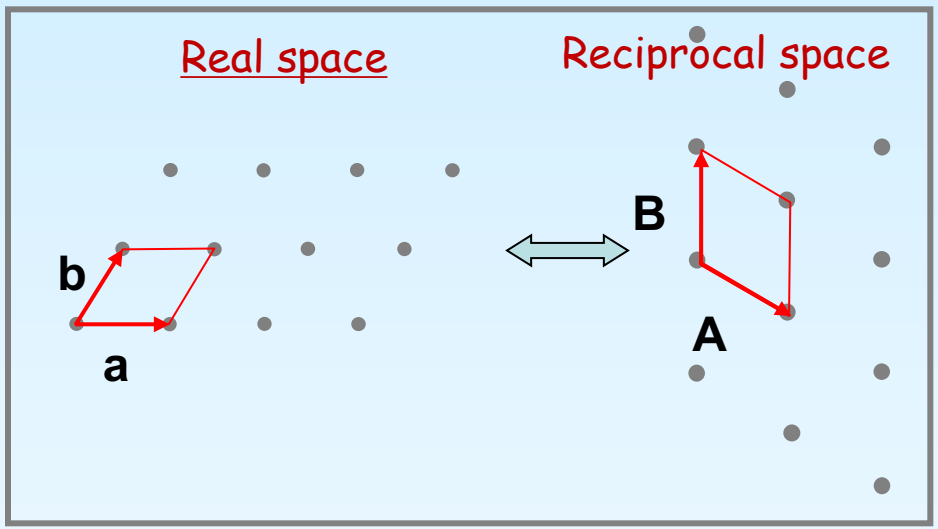


$\Omega = \vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)$ ——volume of primitive unit cell

$\Omega^* = \vec{b}_1 \cdot (\vec{b}_2 \times \vec{b}_3)$ ——volume in the reciprocal lattice

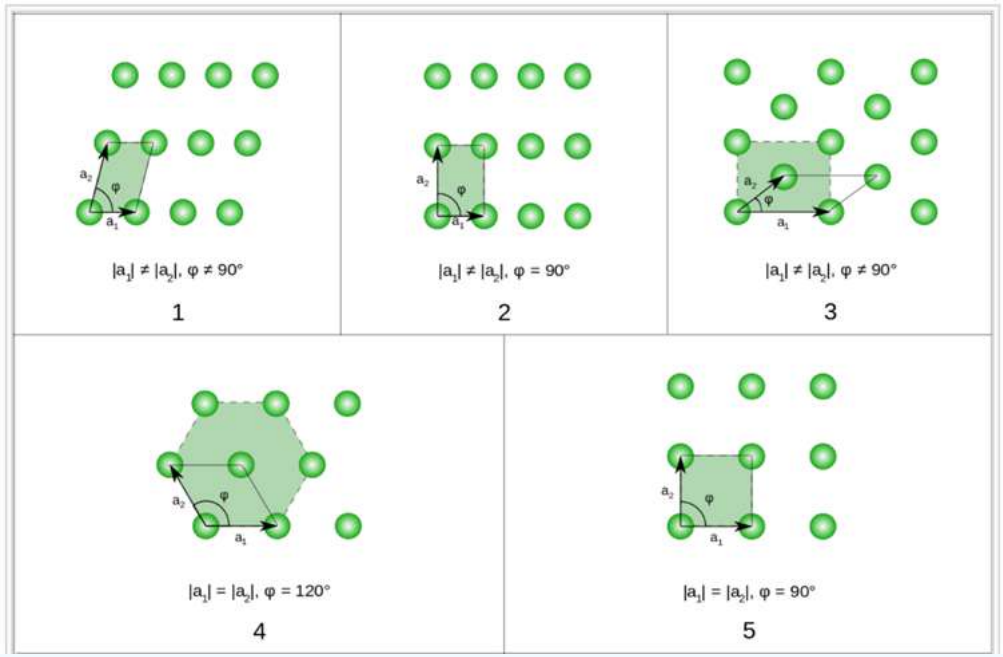
2D reciprocal lattice



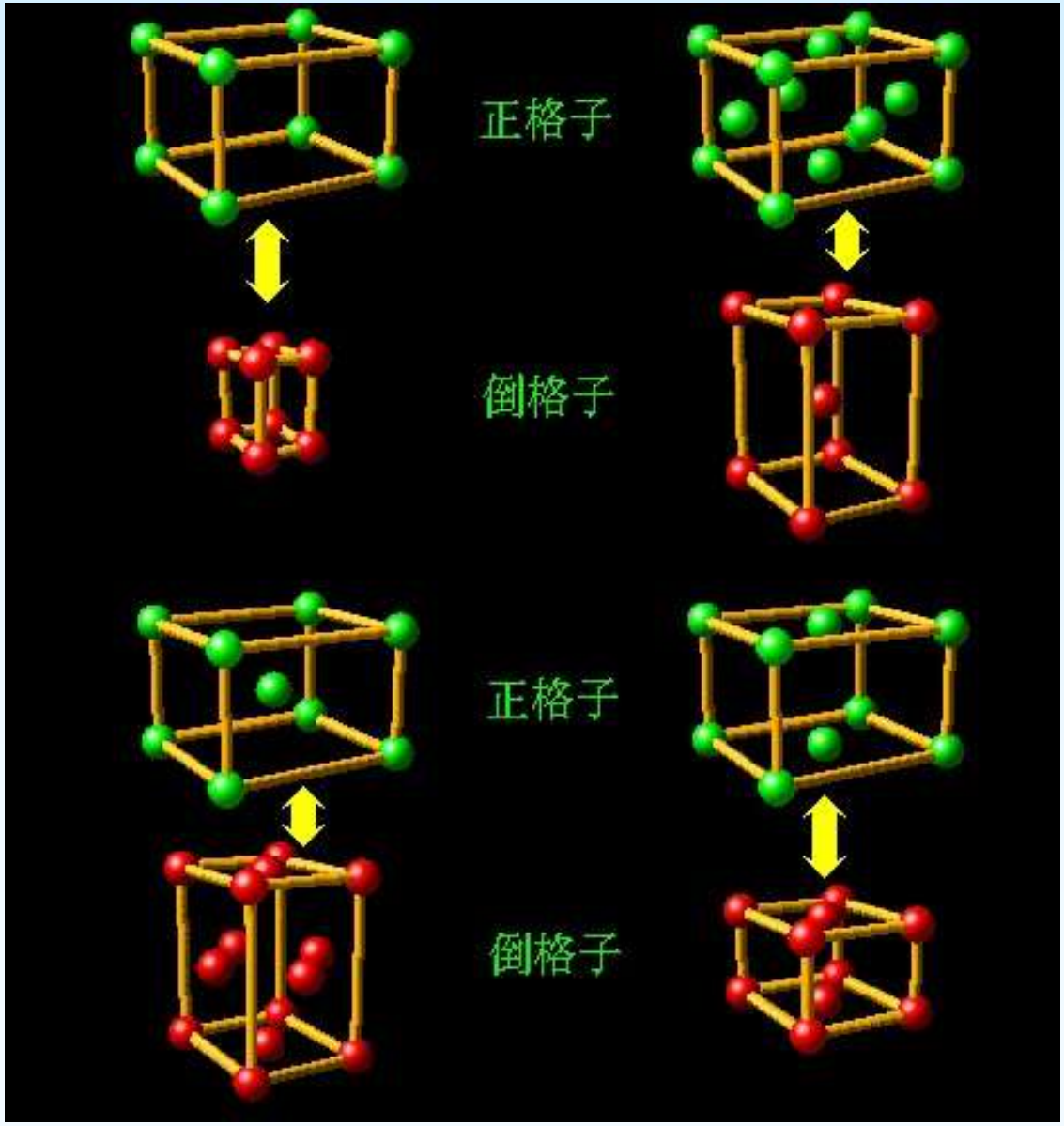


All possible Bravais lattice in 2D:

1. oblique (C_2)
2. rectangular (D_2)
3. face-centered rectangular
4. triangular
5. square

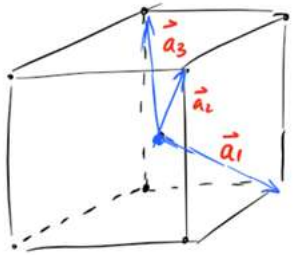


2.1 Reciprocal Lattice



2.1 Reciprocal Lattice

BCC



$$\vec{a}_1 = \frac{a}{2}(\vec{i}+\vec{j}-\vec{k})$$

$$\vec{a}_2 = \frac{a}{2}(\vec{i}-\vec{j}+\vec{k})$$

$$\vec{a}_3 = \frac{a}{2}(-\vec{i}+\vec{j}+\vec{k})$$

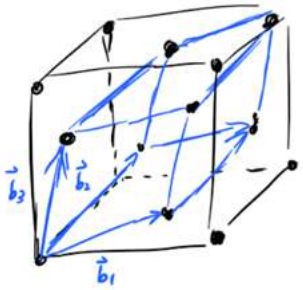
$$\vec{a}_m \cdot \vec{b}_n = 2\pi\delta_{m,n}$$

FCC

$$\vec{b}_1 = \frac{4\pi}{a}(\vec{i}+\vec{j})$$

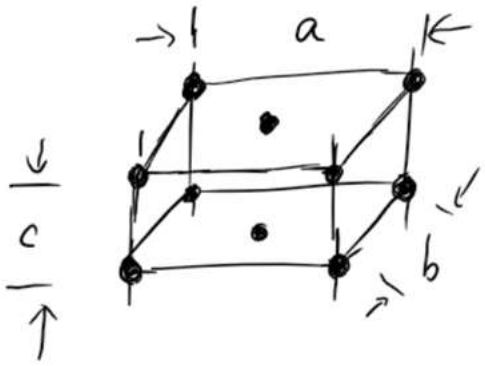
$$\vec{b}_2 = \frac{4\pi}{a}(\vec{i}+\vec{k})$$

$$\vec{b}_3 = \frac{4\pi}{a}(\vec{j}+\vec{k})$$

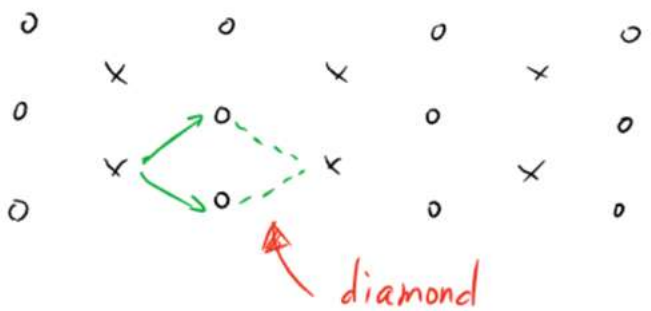


othorhombic (base centered)

[not monoclinic]



⇒



II. Relation between direct and reciprocal lattices

1. The primitive unit cell

volume of primitive cell in reciprocal lattice:

$$\Omega^* = \frac{(2\pi)^3}{\Omega}$$

$$\Omega^* = \vec{b}_1 \cdot (\vec{b}_2 \times \vec{b}_3) = \frac{(2\pi)^3}{\Omega^3} (\vec{a}_2 \times \vec{a}_3) \cdot [(\vec{a}_3 \times \vec{a}_1) \times (\vec{a}_1 \times \vec{a}_2)]$$

$$\vec{A} \times (\vec{B} \times \vec{C}) = (\vec{A} \cdot \vec{C})\vec{B} - (\vec{A} \cdot \vec{B})\vec{C} = \Omega \vec{a}_1$$

$$\Omega^* = \frac{(2\pi)^3}{\Omega^3} (\vec{a}_2 \times \vec{a}_3) \cdot \Omega \vec{a}_1 = \frac{(2\pi)^3}{\Omega}$$

2.1 Reciprocal Lattice

2. lattice plane and the family of lattice planes

In a given Bravais lattice, a lattice plane is defined to be any plane containing infinitely many lattice sites.

⇒ Any lattice plan in a 3D Bravais lattice is a 2D Bravais lattice.

By a family of lattice planes we mean a set of parallel, equally spaced lattice planes, which together contain all the points of the 3D Br. latt.

3. Relation of reciprocal lattice vector to a family of direct lattice planes

Theorem For any family of planes separated by a distance d, there are reciprocal lattice vectors perpendicular to the planes, the shortest of which have a length $2\pi/d$.

2.1 Reciprocal Lattice

Conversly For any reciprocal lattice vector $\vec{K}$, there is a family of planes normal to $\vec{K}$, seperated by distance d, where $2\pi/d$ is the shortest length of reciprocal lattice vector parallel to $\vec{K}$.

2.1 Reciprocal Lattice

- Use reciprocal lattice vector to index the family of lattice planes

$\vec{K} = h\vec{b}_1 + k\vec{b}_2 + l\vec{b}_3$ and plane (h,k,l)

Use Miller index (h,k,l) to label the family of planes (h,k,l)

$$e^{i\vec{K}\cdot\vec{R}} = 1 \Rightarrow \vec{K}\cdot\vec{R} = A \Rightarrow \vec{K}\cdot\vec{a}_1 x_1 = \vec{K}\cdot\vec{a}_2 x_2 = \vec{K}\cdot\vec{a}_3 x_3$$

$$\Rightarrow x_1 \cdot h = x_2 k = x_3 l$$

$$\Rightarrow x_1 = A/h,\ x_2 = A/k,\ x_3 = A/l$$

intercepts are inversely proportional to h, k, l.

III. Brillouin zone, BZ

The Wigner-Seitz primitive unit cell of the reciprocal lattice is called the *first* Brillouin zone.

Example 1. 2D square lattice

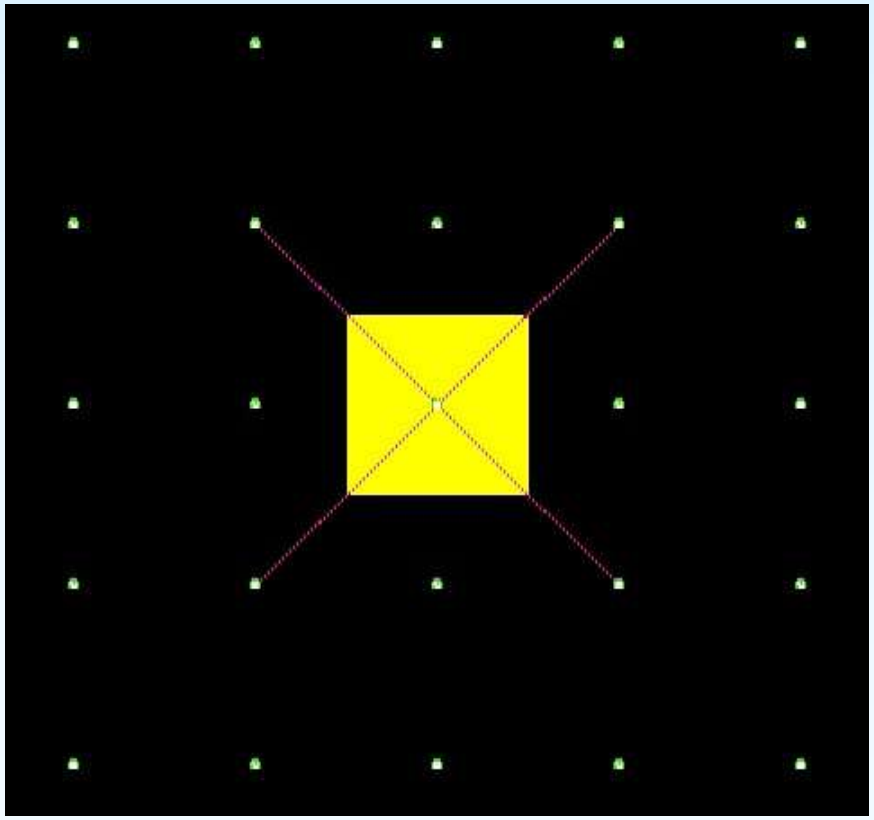
direct lattice: $\vec{a}_1 = a\vec{i}$ $\vec{a}_2 = a\vec{j}$

reciprocal lattice: $\vec{b}_1 = \frac{2\pi}{a}\vec{i}$ $\vec{b}_2 = \frac{2\pi}{a}\vec{j}$

2.1 Reciprocal Lattice

first BZ:

$$\vec{G}_{11} = \vec{b}_1$$
$$\vec{G}_{12} = \vec{b}_2$$
$$\vec{G}_{13} = -\vec{b}_1$$
$$\vec{G}_{14} = -\vec{b}_2$$



2.1 Reciprocal Lattice

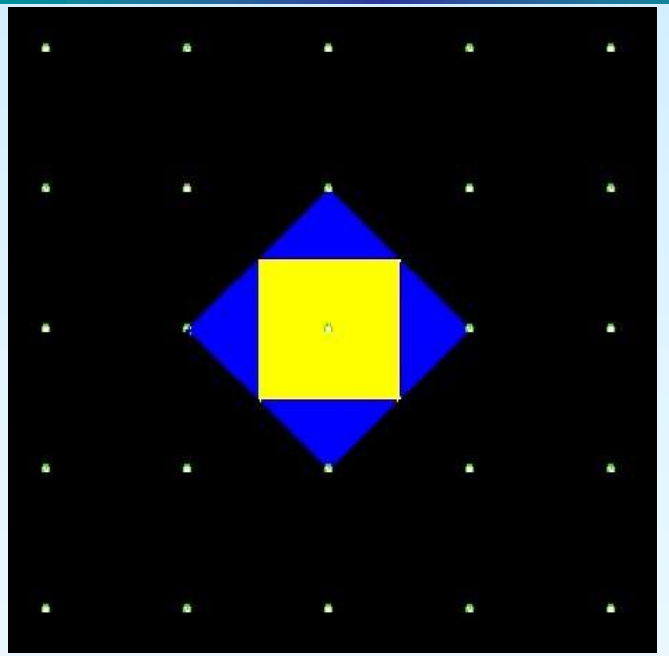
2nd BZ :

$$\vec{G}_{21} = \vec{b}_1 + \vec{b}_2$$

$$\vec{G}_{22} = \vec{b}_1 - \vec{b}_2$$

$$\vec{G}_{23} = -\vec{b}_1 + \vec{b}_2$$

$$\vec{G}_{24} = -\vec{b}_1 - \vec{b}_2$$



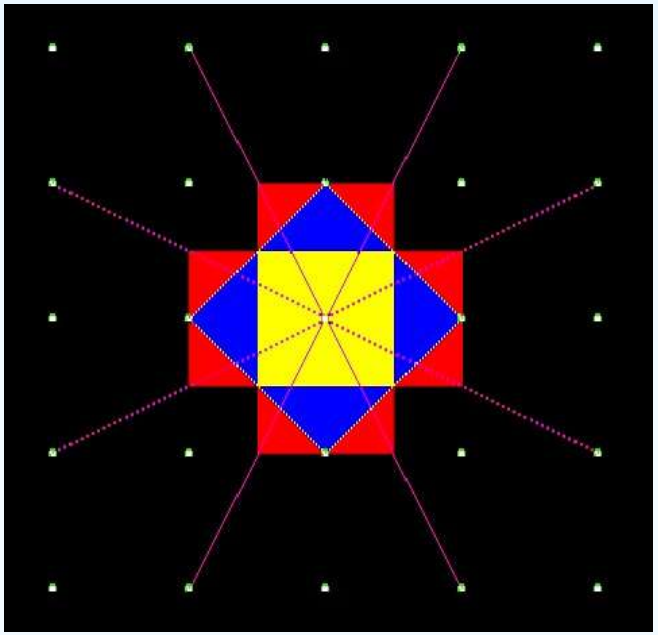
3rd BZ :

$$\vec{G}_{31} = 2\vec{b}_1$$

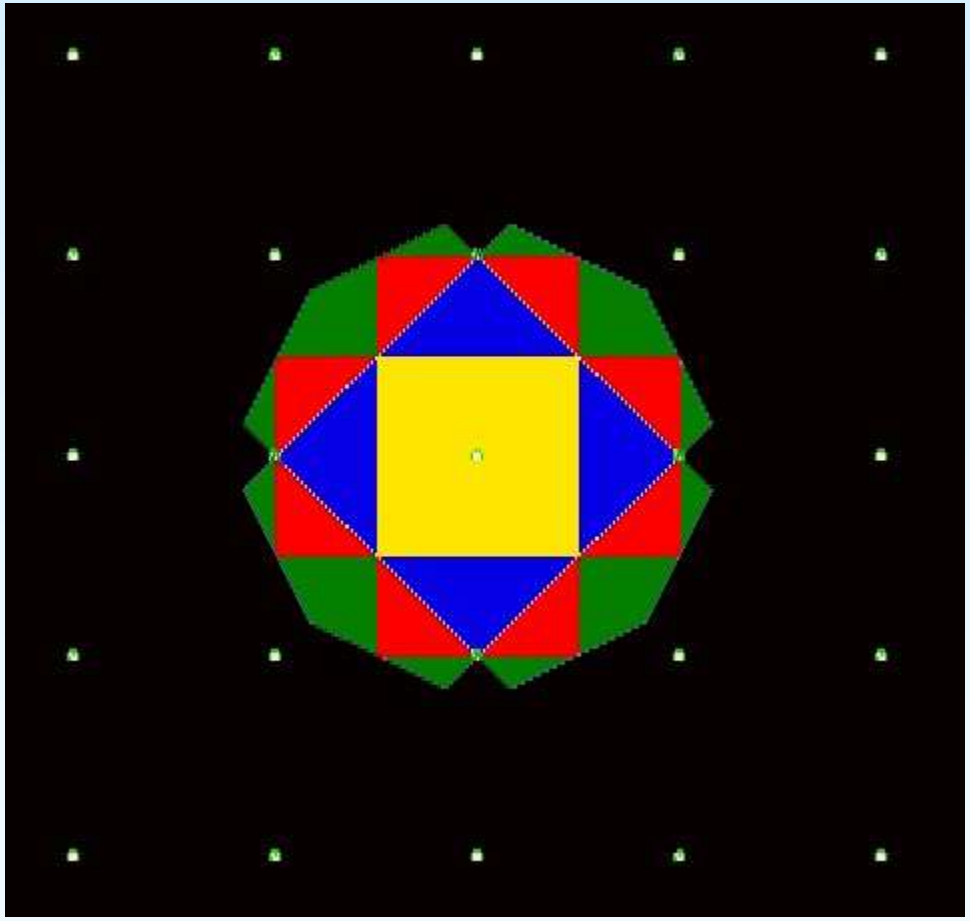
$$\vec{G}_{32} = 2\vec{b}_2$$

$$\vec{G}_{33} = -2\vec{b}_1$$

$$\vec{G}_{34} = -2\vec{b}_2$$



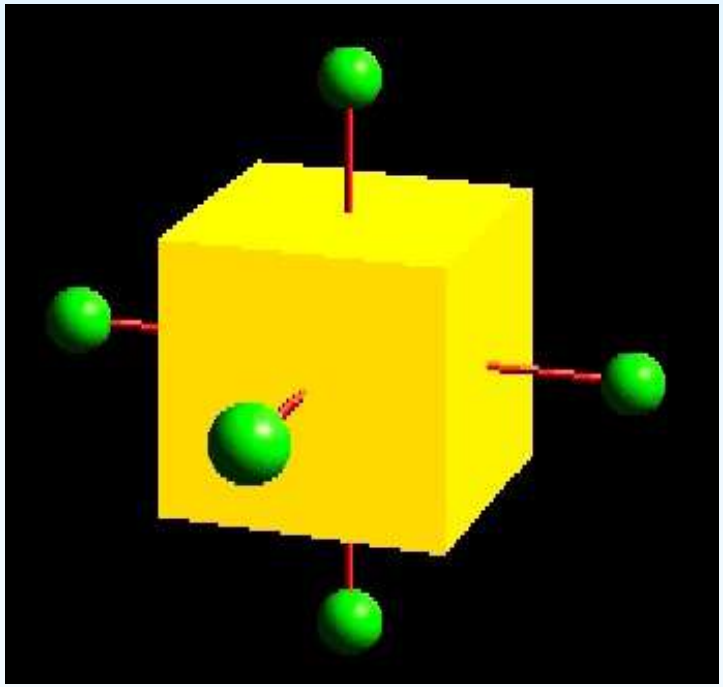
2.1 Reciprocal Lattice



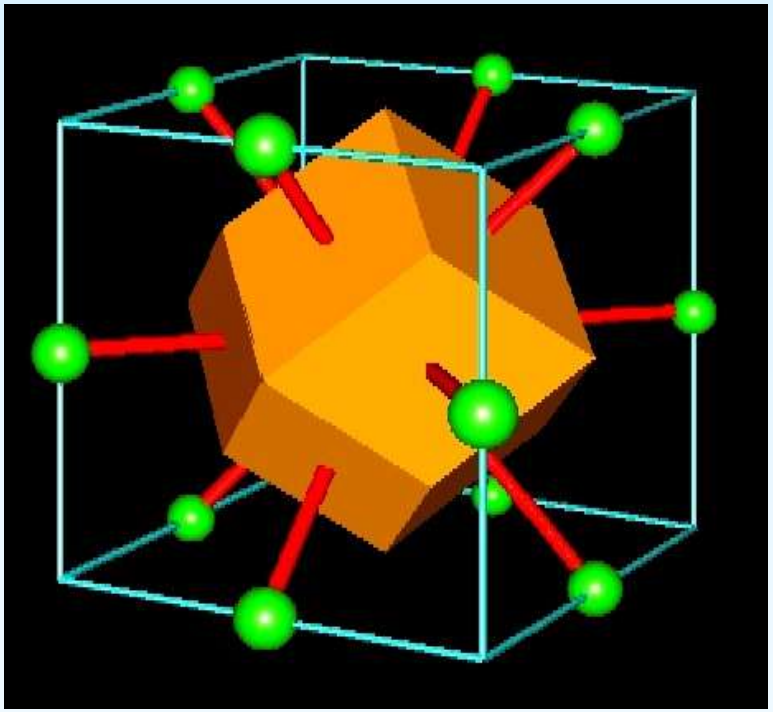
Example 2. Simple Cubic

$$\vec{a}_1 = a\vec{i} \qquad \vec{a}_2 = a\vec{j} \qquad \vec{a}_3 = a\vec{k}$$

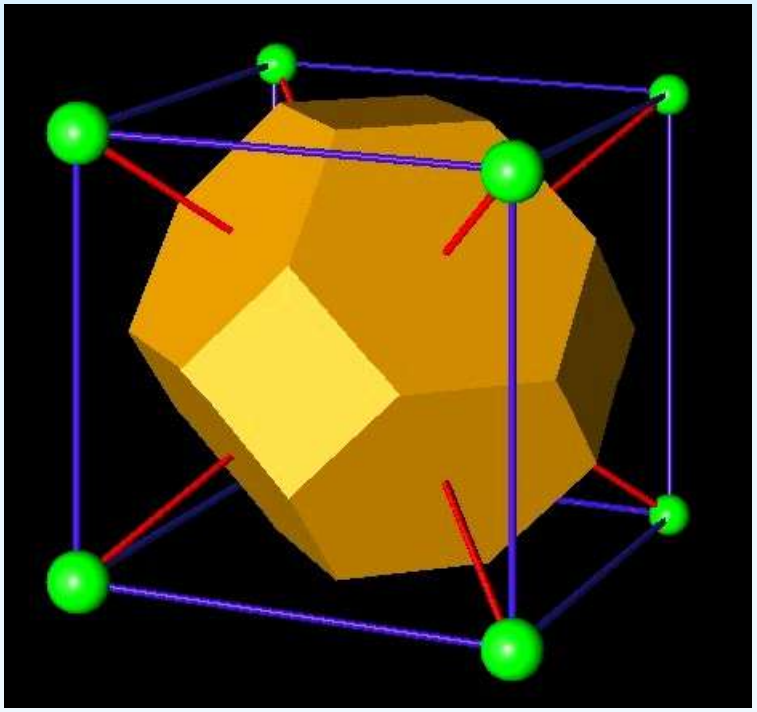
$$\vec{b}_1 = \frac{2\pi}{a}\vec{i} \qquad \vec{b}_2 = \frac{2\pi}{a}\vec{j} \qquad \vec{b}_3 = \frac{2\pi}{a}\vec{k}$$



Example 3. BCC & FCC



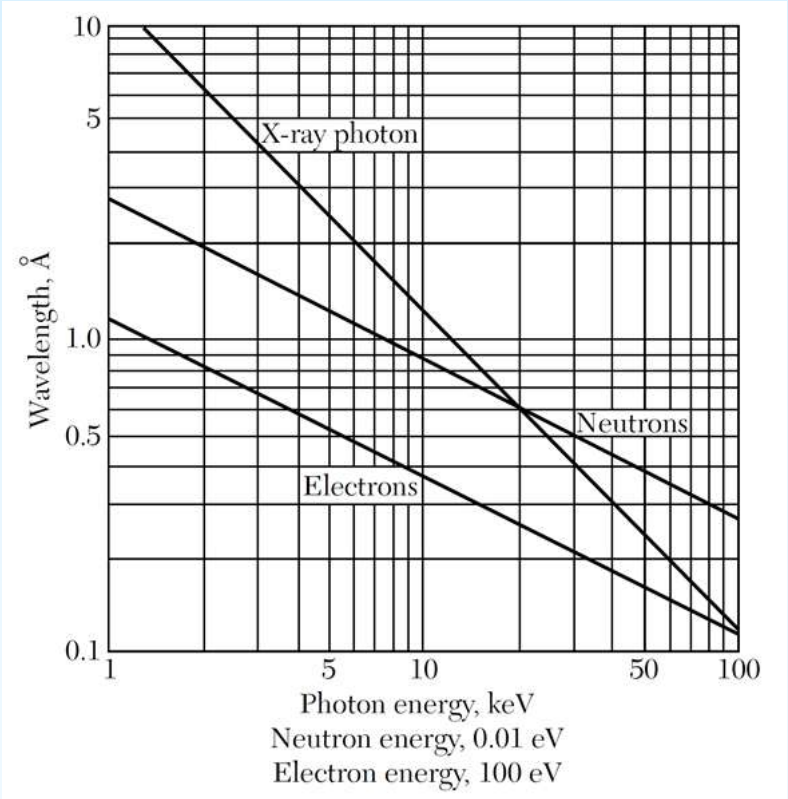
1st BZ of BCC



1st BZ of FCC

2.2 Experimental determination of crystal structures

- ✓ **Study the crystal structure by diffractions of *waves*.**
- ✓ **3 kinds of waves: photon, electron, and nuetron.**
- ✓ **The crystalline atoms cause a beam of incident X-rays to diffract into many specific directions.**
- ✓ ***Diffracted beams in directions quite different from the incident direction!***

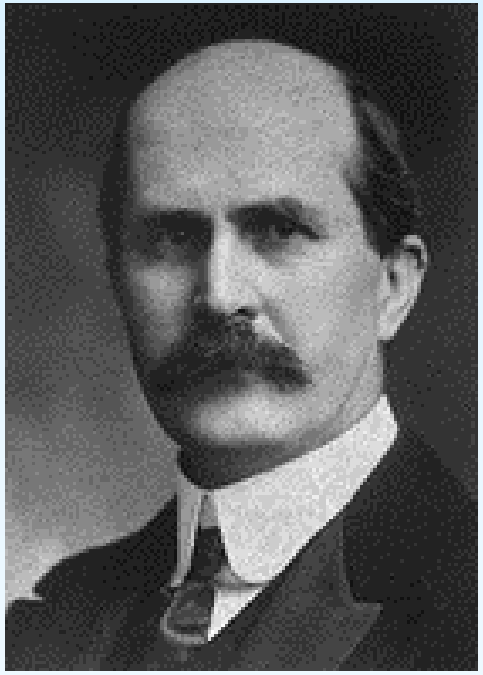


Wavelength versus particle energy, for photons, neutrons, and electrons.

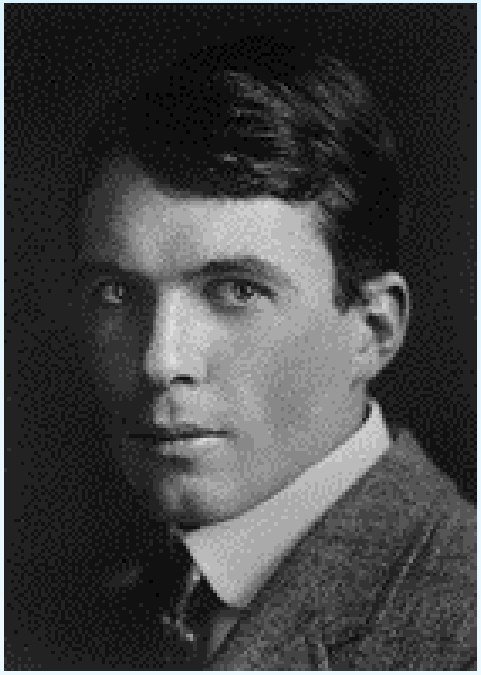
I. X-Ray Crystalography

Max von Laue
1914

The Nobel Prize in Physics 1914 was awarded to Max von Laue *"for his discovery of the diffraction of X-rays by crystals".*



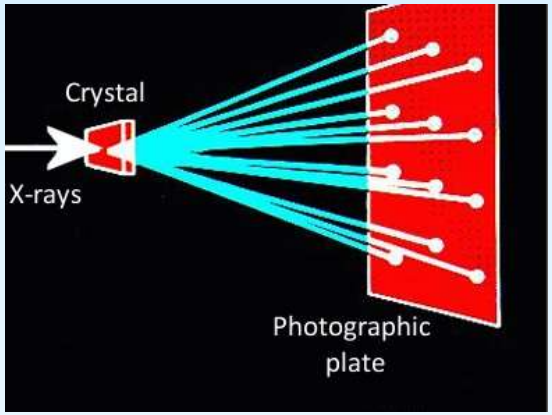
William Henry Bragg
1915



William Lawrence Bragg
1915

The Nobel Prize in Physics 1915 was awarded jointly to Sir William Henry Bragg and William Lawrence Bragg "*for their services in the analysis of crystal structure by means of X-rays*"

1.5 Experimental determination of crystal structures



June 8th 2012 marks the **100th anniversary** **of the first report of X-ray diffraction by Max von Laue and colleagues**, **University of Munich, Germany**.

von Laue came up with the idea to send a beam of X-rays through a copper sulfate crystal and record the results on photographic plates (pictured).

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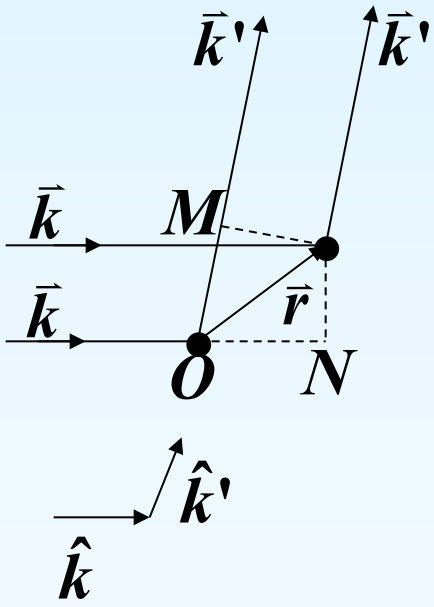
(1) Diffraction Conditions (Laue condition)

Theorem: The set of reciprocal lattice vectors G determines the possible x-ray reflections.



path length diff.: $\delta = ON - OM = \vec{r}\cdot\hat{k} - \vec{r}\cdot\hat{k}'$

constructive cond.: $\vec{r}\cdot(\hat{k}-\hat{k}') = n\lambda$, *n is integer*

The incident & reflected wave:

$$\vec{k} = \frac{2\pi}{\lambda}\hat{k} \qquad \vec{k}' = \frac{2\pi}{\lambda}\hat{k}'$$

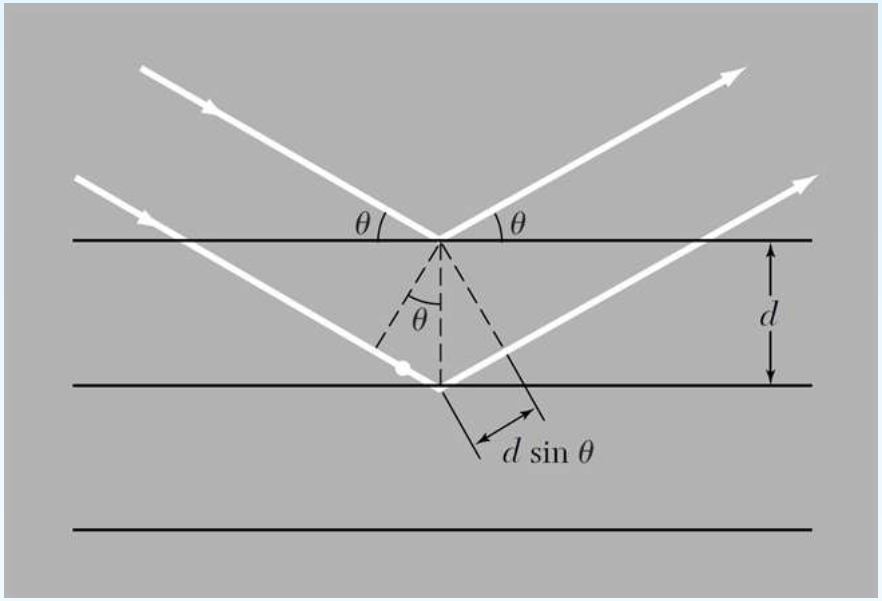
$$\frac{\lambda}{2\pi}\vec{r}\cdot(\vec{k}-\vec{k}') = n\lambda \qquad \boxed{\vec{r}\cdot(\vec{k}-\vec{k}') = 2\pi n}$$

$\vec{r}$: direct lattice vector, $\vec{R}_n\cdot\vec{G}_h = 2\pi m$ ⇒

$\boxed{\vec{k}-\vec{k}' = \vec{G}_h}$ ——Diffr. Cond. in the reciprocal lattice

(2) Bragg law

- ✓ **3D Bravais latt. can be decomposed into a family of lattice planes.**
- ✓ **X-ray beams are reflected on the planes and have constructive or distructive interferances according to the phase factors.**



path diff.: $\delta = 2d\sin\theta$

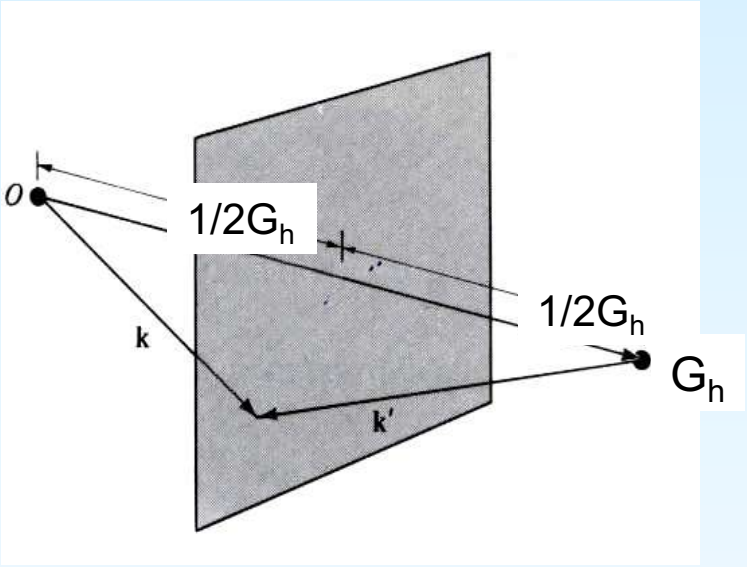
$$n\lambda = 2d\sin\theta$$

$n = 1, 2, 3, \cdots$ **order of diffr.**

——Bragg condition

Bragg law can be satisfied only for wavelength $\lambda \leqq 2d$

(3) Derive the Bragg condition from Laue condition



diffr. cond. in reciprocal space

$$\vec{k}-\vec{k}'=\vec{G}_h \qquad |\vec{k}|=|\vec{k}'|=\frac{2\pi}{\lambda}$$

$\vec{k},\vec{k}',\vec{G}_h$ constitutes an isosceles

$\vec{G}_h$ is perpendicular to the Bragg plane $(h_1h_2h_3)$

The Laue diffraction can be regarded as Bragg reflection from $\vec{k}$ to $\vec{k}'$ on the crystal plane $(h_1h_2h_3)$, since $|G|=2\pi/d$:

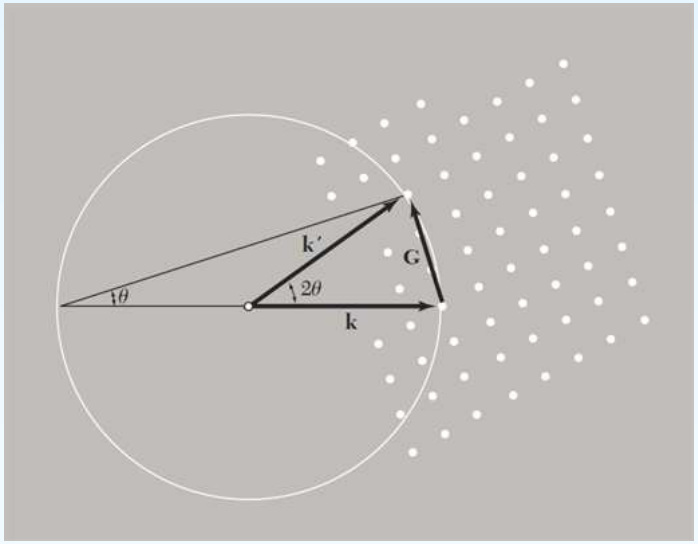
diffr. cond. in direct space

$$|\vec{k}|=|\vec{k}'|=\frac{|\vec{G}_h|}{2\sin\theta}=\frac{2\pi n}{2d\sin\theta} \Rightarrow 2d\sin\theta=n\lambda$$

(4) Laue Equations and Ewald Construction

$$\mathbf{a}_1 \cdot \Delta\mathbf{k} = 2\pi v_1 \ ; \qquad \mathbf{a}_2 \cdot \Delta\mathbf{k} = 2\pi v_2 \ ; \qquad \mathbf{a}_3 \cdot \Delta\mathbf{k} = 2\pi v_3 \ .$$

Laue equations, **hard** to be satisfied simultaneously!

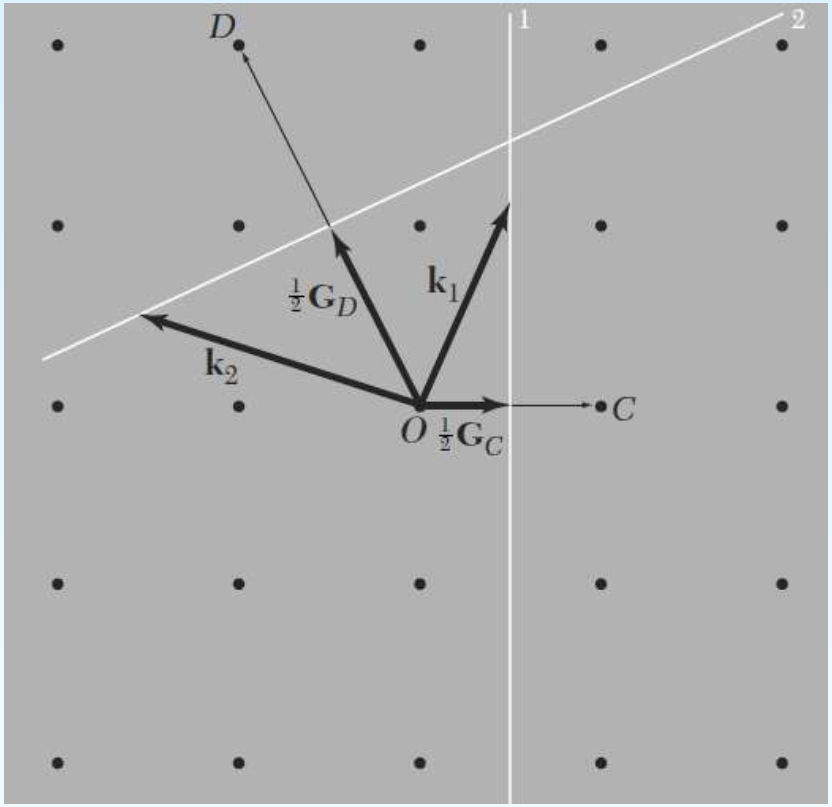


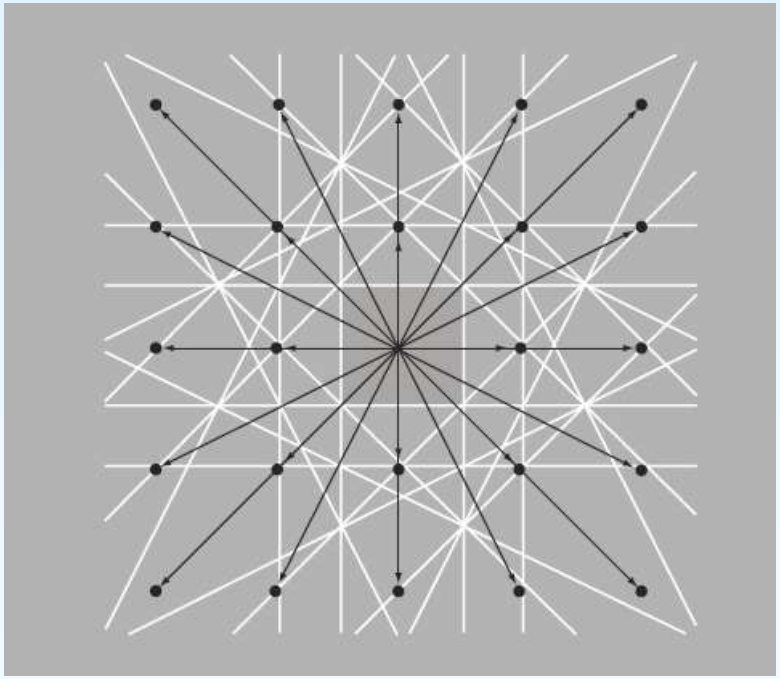
- ✓ The points on the right-hand side are reciprocal-lattice points of the crystal. k terminates at any reciprocal lattice point.
- ✓ A diffracted beam will be formed if this sphere intersects any other point in the reciprocal lattice.

This construction is due to P. P. Ewald

(5) Brillouin zones and Diffraction Condition

$$\mathbf{k} \cdot \left(\frac{1}{2}\mathbf{G}\right) = \left(\frac{1}{2}G\right)^2$$





The Brillouin zone gives a vivid geometrical interpretation of the diffraction condition.

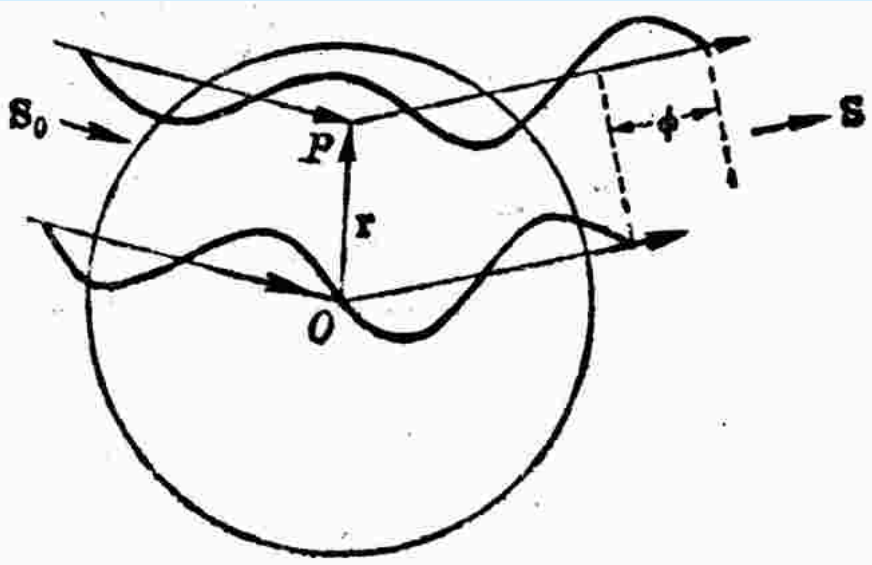
2. Structure Factor

- ✓ **Laue Eq. & Bragg Cond. — determine the planes/directions having significant constructive diffraction.**
- ✓ **Structure Factor — determine the intensity of diffraction.**

- ✓ **Fourier Transform of a periodic function on a lattice**

$$n(\mathbf{r}) = \sum_{\mathbf{G}} n_{\mathbf{G}} \exp(i\mathbf{G}\cdot\mathbf{r})$$

$$n_{\mathbf{G}} = V_c^{-1} \int_{\text{cell}} dV\, n(\mathbf{r}) \exp(-i\mathbf{G}\cdot\mathbf{r})$$



$\vec{r}$ is the position vector of point ***P***, the phase diff. of the scattered wave from point ***P*** with that from origin point ***O*** is :

$$\Delta\varphi = \left(\vec{k}' - \vec{k}\right)\cdot\vec{r}$$

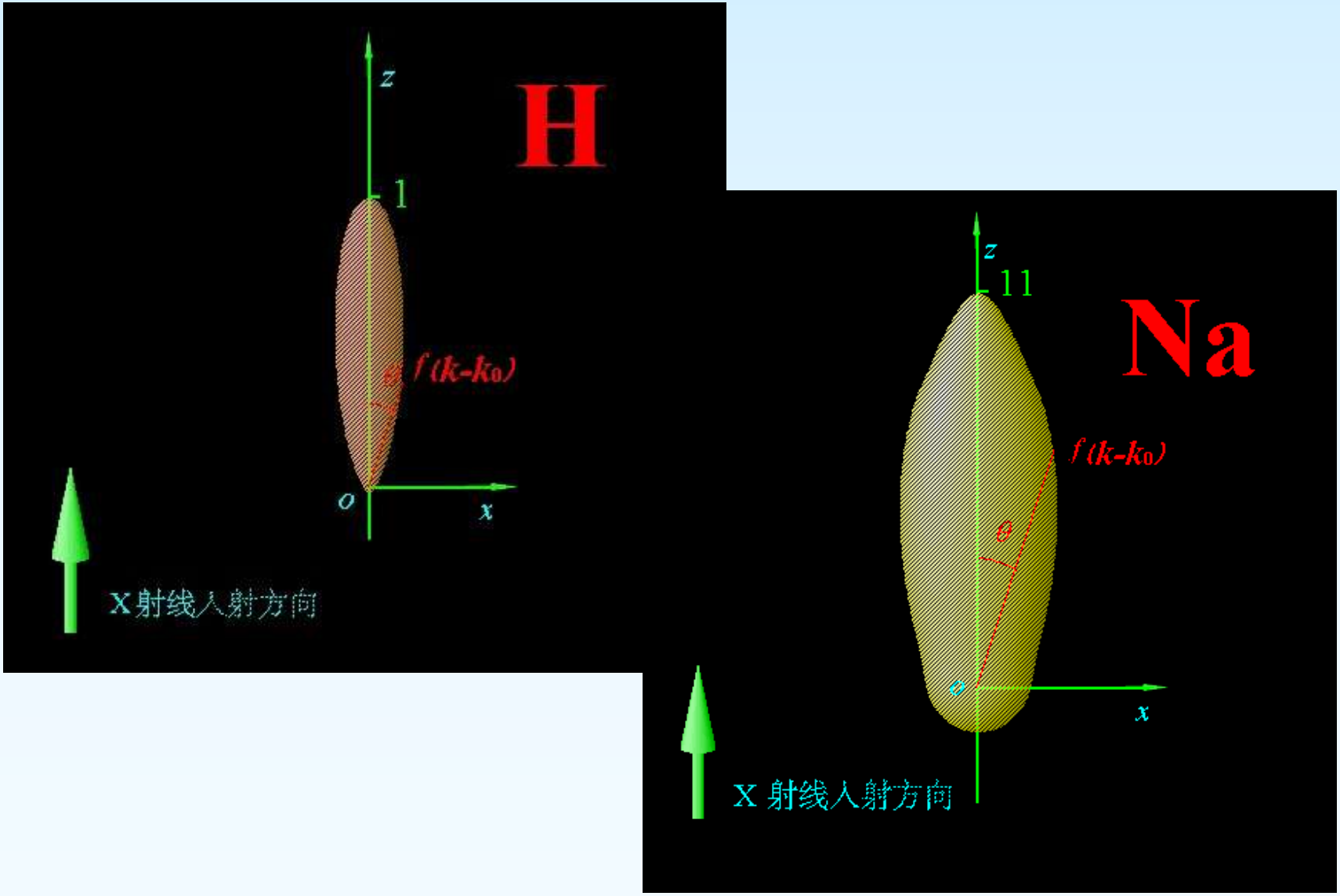
electron density around an atom j: $n_j(\vec{r})$

Total scattering amplitude along $\vec{k}'$ direction:

$$f_j\left(\vec{G}_h\right) = \int n_j(\vec{r})\, e^{i\left(\vec{k}'-\vec{k}\right)\cdot\vec{r}}\, \mathrm{d}\vec{r} = \int n_j(\vec{r})\, e^{-i\vec{G}_h\cdot\vec{r}}\, \mathrm{d}\vec{r}$$

——Atomic form factor, measuring the scattering ability of a single atom

2.2 Experimental determination of crystal structures



(2) Geometrical Structure Factor

Consider *p* atoms with position vectors:

$$\vec{d}_j, \quad j = 1, 2, \cdots, p$$

Phase diff. of scattered wave from $\vec{d}_j$ with that from origin:

$$\Delta\varphi = \left(\vec{k}' - \vec{k}\right) \cdot \vec{d}_j$$

Total scattering amplitude (of a unit cell) along $\vec{k}'$ direction:

$$S_{\vec{G}_h} = f\left(\vec{G}_h\right) \sum_{j=1}^{p} e^{-i\vec{G}_h \cdot \vec{d}_j}$$

——**geometrical structure factor**

atom form factor, atom arrangement, diffraction direction

(3) Cancellation Condition:

diffraction intensity: $I_{hkl} \propto \left|S_{\vec{G}_h}\right|^2 = S^*_{\vec{G}_h} \cdot S_{\vec{G}_h}$

Peak disappears in the diffraction pattern when I=0.

① BCC

Conventional unit cell of BCC contains *two* atoms:

$$\vec{d}_1 = 0 \qquad \vec{d}_2 = \frac{1}{2}a(\hat{x}+\hat{y}+\hat{z}) \qquad f_1 = f_2 = f$$

$$\vec{G}_h = h_1\vec{b}_1 + h_2\vec{b}_2 + h_3\vec{b}_3 = \frac{2\pi}{a}(h_1\hat{x} + h_2\hat{y} + h_3\hat{z})$$

$$S_{\vec{G}_h} = \sum_{j=1}^{p} f_j\left(\vec{G}_h\right) e^{-i\vec{G}_h\cdot\vec{d}_j}$$

$$S(\vec{G}_h) = f\left[1+\mathrm{e}^{-i\pi(h_1+h_2+h_3)}\right]$$

$$= \begin{cases} 0 & \text{当} h_1+h_2+h_3 = \text{奇数} \\ 2f & \text{当} h_1+h_2+h_3 = \text{偶数} \end{cases}$$

Family of lattice planes having diffraction peaks: （110）（200）（211）…

② FCC

Conventional unit cell of BCC contains *four* atoms:

$$\vec{d}_1 = 0 \quad \vec{d}_2 = \frac{1}{2}a(\hat{x}+\hat{y}) \quad \vec{d}_3 = \frac{1}{2}a(\hat{y}+\hat{z}) \quad \vec{d}_4 = \frac{1}{2}a(\hat{x}+\hat{z})$$

$$f_1 = f_2 = f_3 = f_4 = f$$

$$\vec{G}_h = h_1\vec{b}_1 + h_2\vec{b}_2 + h_3\vec{b}_3 = \frac{2\pi}{a}(h_1\hat{x}+h_2\hat{y}+h_3\hat{z})$$

2.2 Experimental determination of crystal structures

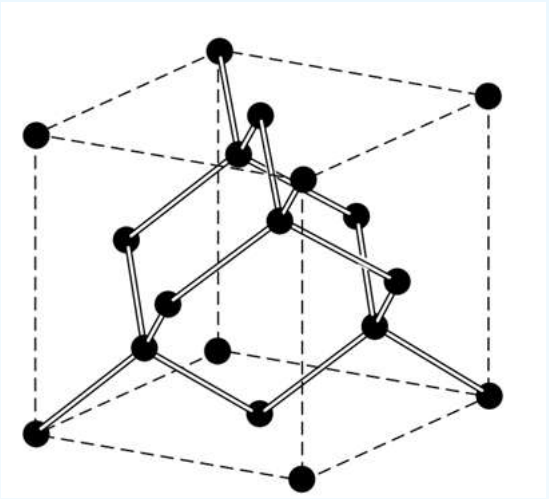
$$S(\vec{G}_h) = f\left[1+e^{-i\pi(h_1+h_2)}+e^{-i\pi(h_2+h_3)}+e^{-i\pi(h_1+h_3)}\right]$$

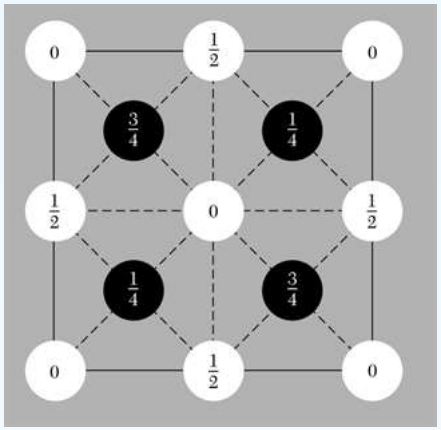
$$= \begin{cases} 0 & \text{当} h_1, h_2, h_3 \text{部分为奇,部分为偶时} \\ 4f & \text{当} h_1, h_2, h_3 \text{全为奇数或全偶数时} \end{cases}$$

Diffaction peak cancels when the Miller index contains both even and odd numbers; the plane indices consisting of all even or odd numbers show up in the diffraction patern, say: (111), (200), (220)…

③ diamond structure

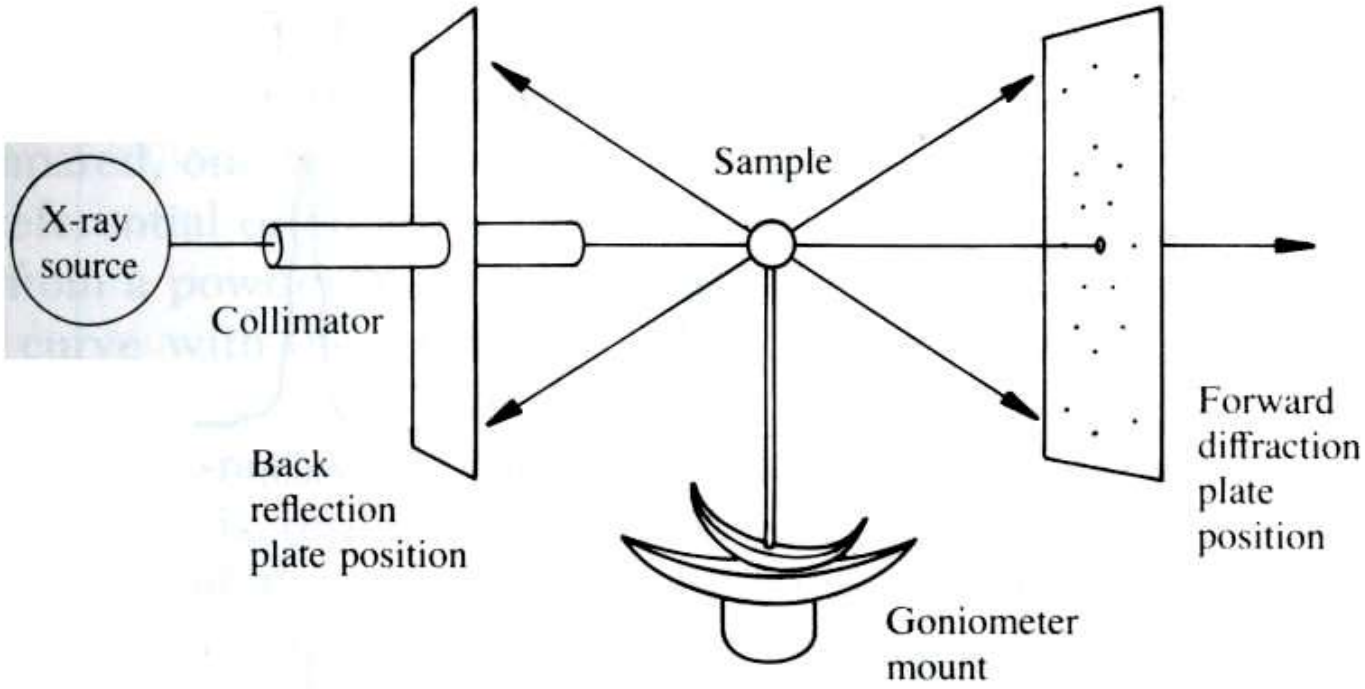
See exercises Ex. 5 of the text book (C. Kittel).





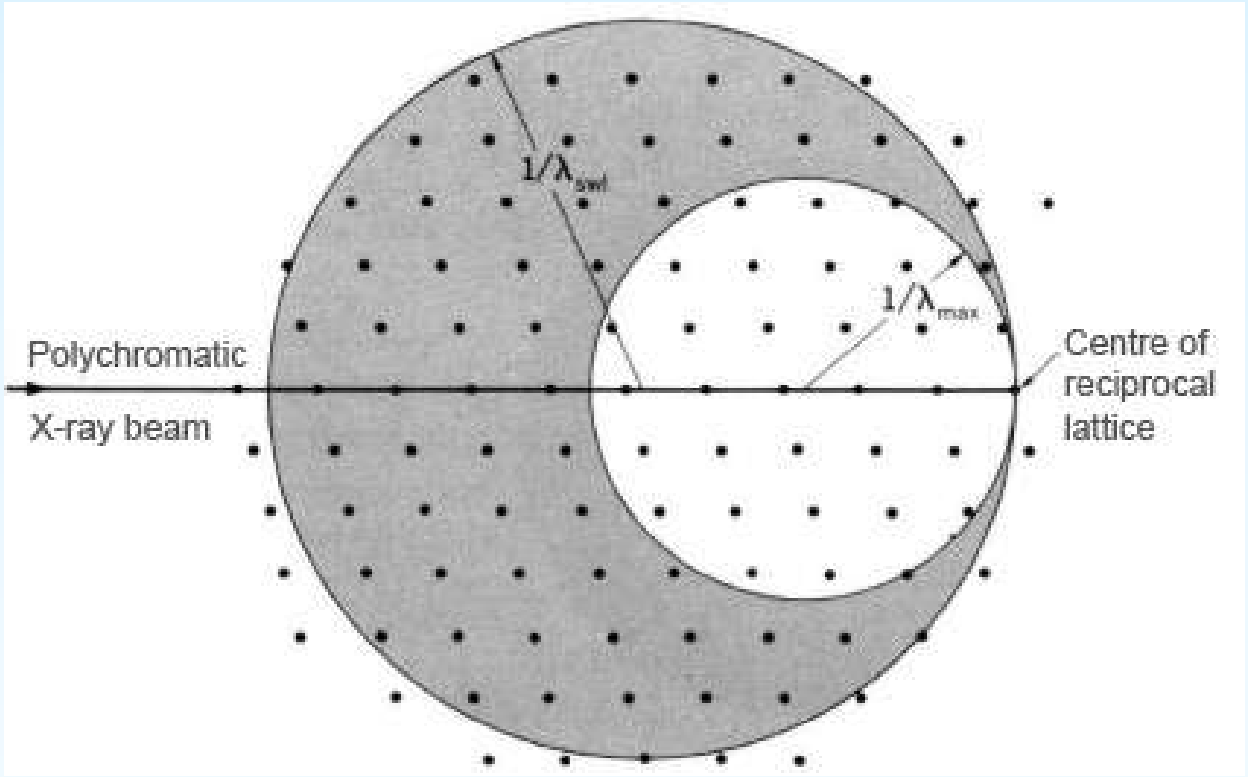
3. Experimental methods of XRD

(1) Laue Method continuous X-ray spectrum



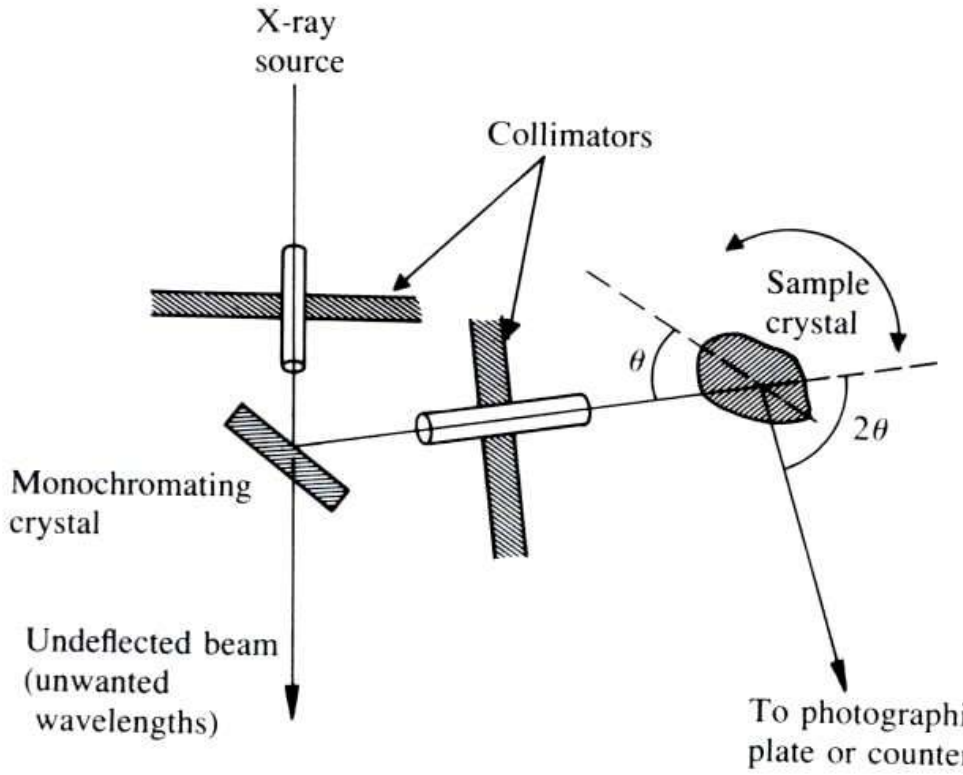
A Laue flat plane camera, using polychromatic X-rays. The pattern of Laue spots can be photographed in either the forward or the back-reflection position. The sample can be rotated about three orthogonal axes, and then X-rayed again, to confirm that a desired orientation has been obtained.

Laue Method


$1/\lambda_{min}$
$1/\lambda_{max}$
Polychromatic
X-ray beam
Centre of
reciprocal
lattice

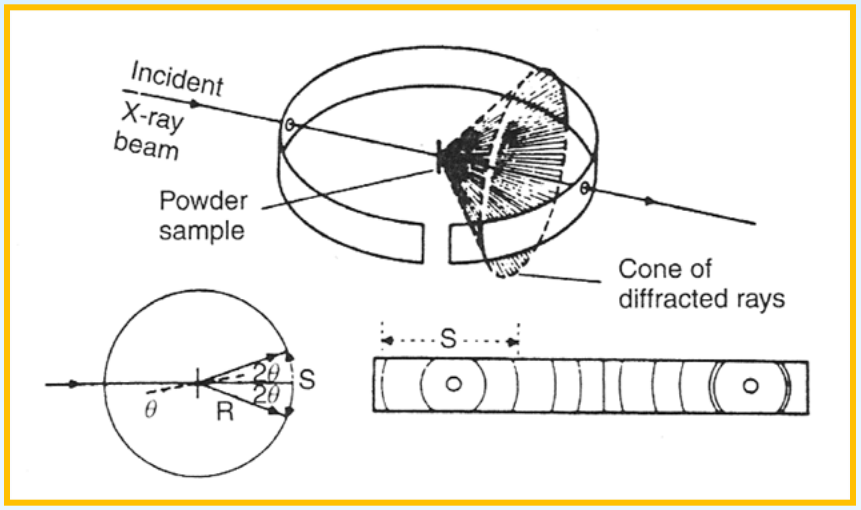
(2) rotating-crystal method

single-frequency X-ray



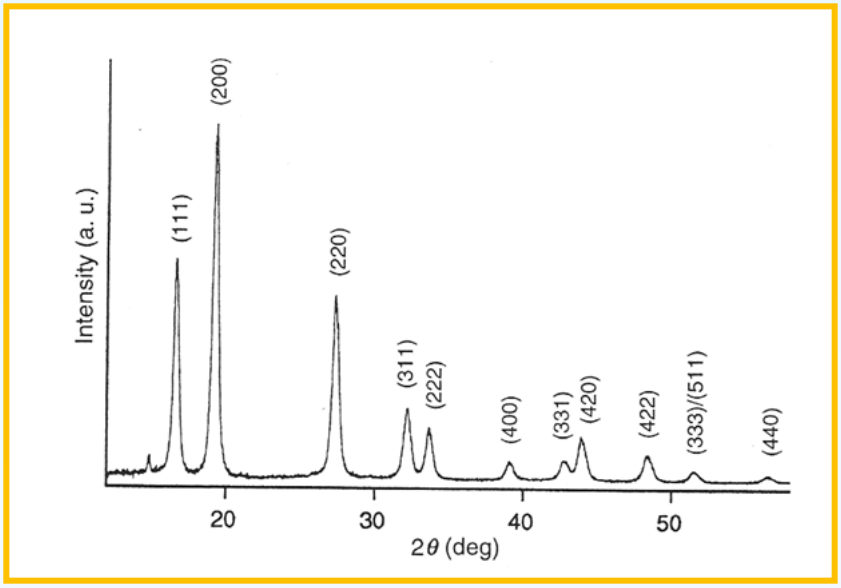
A rotating crystal arrangement, using monochromatic X-rays selected by Bragg reflection from a separate crystal. In a rotating crystal camera, the crystal is rocked back and forth while the series of diffraction images is recorded on a cylinder of photographic film placed so that its axis coincides with the rotation axis.

(3) Powder or Debye method

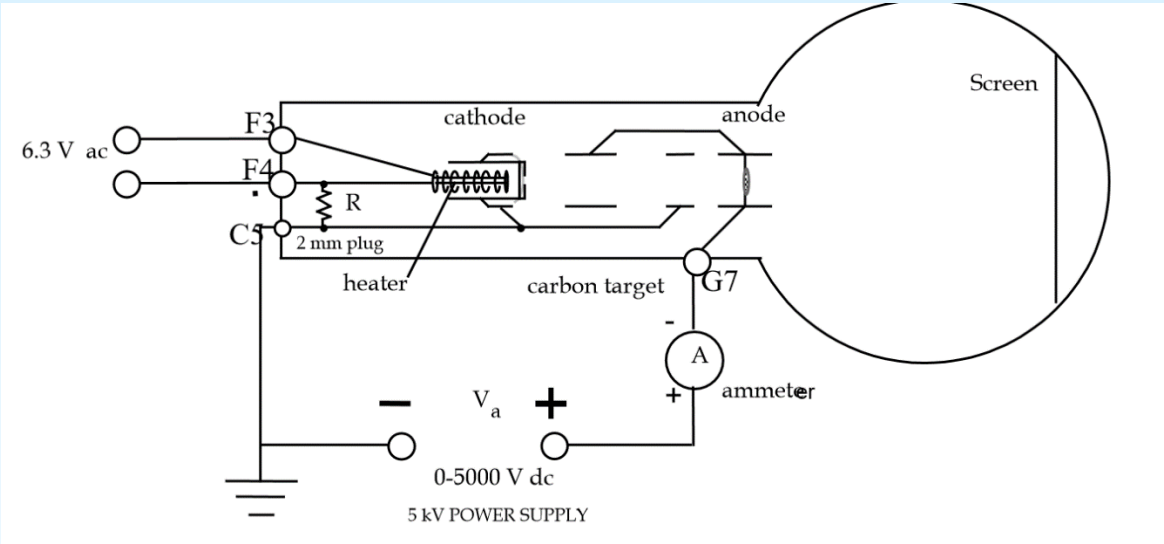


monochromatic X ray,
use powder or polycrystal

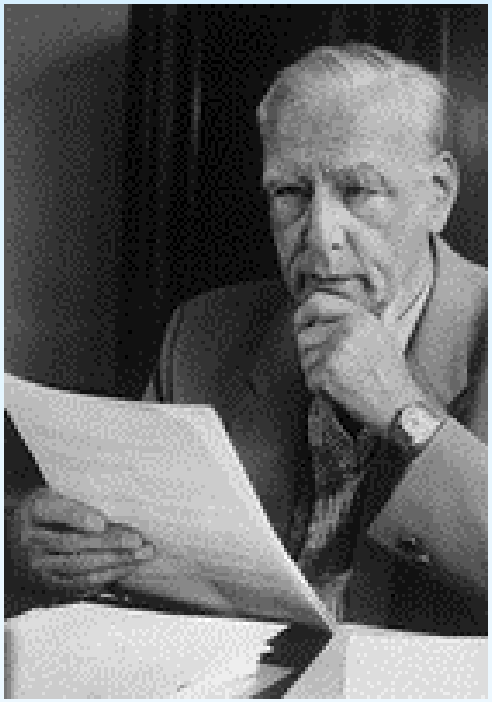
Diffraction pattern of example powder X



II. electron & neutron diffraction



Electron Diffraction Experiment Diagram

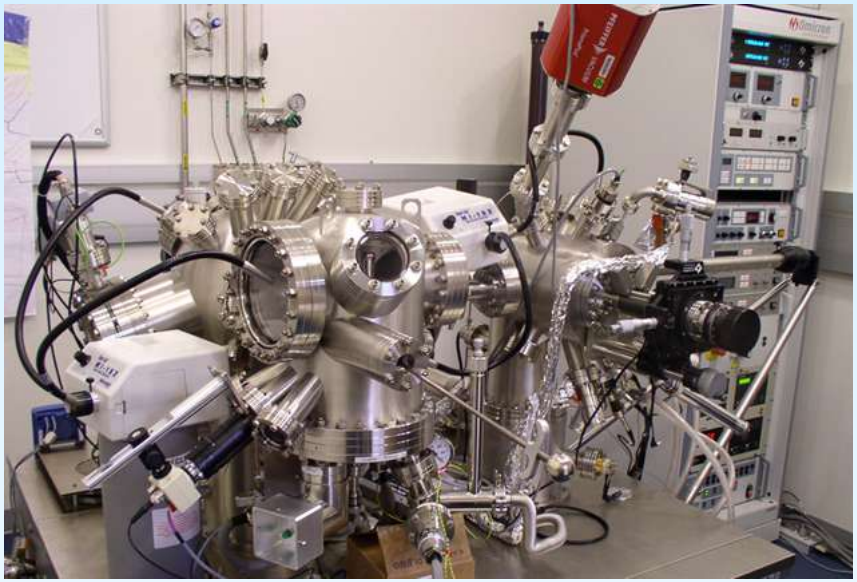


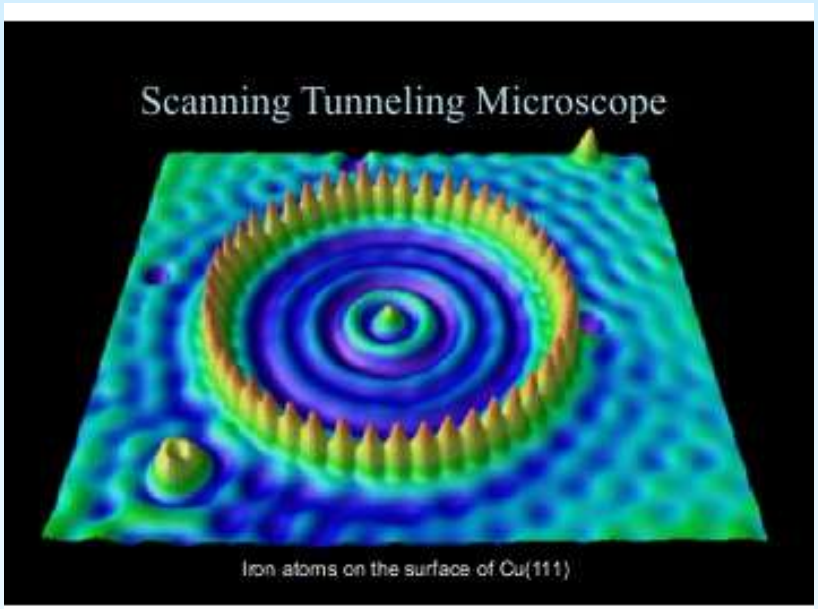
Ernst Ruska
1986, electron microscope

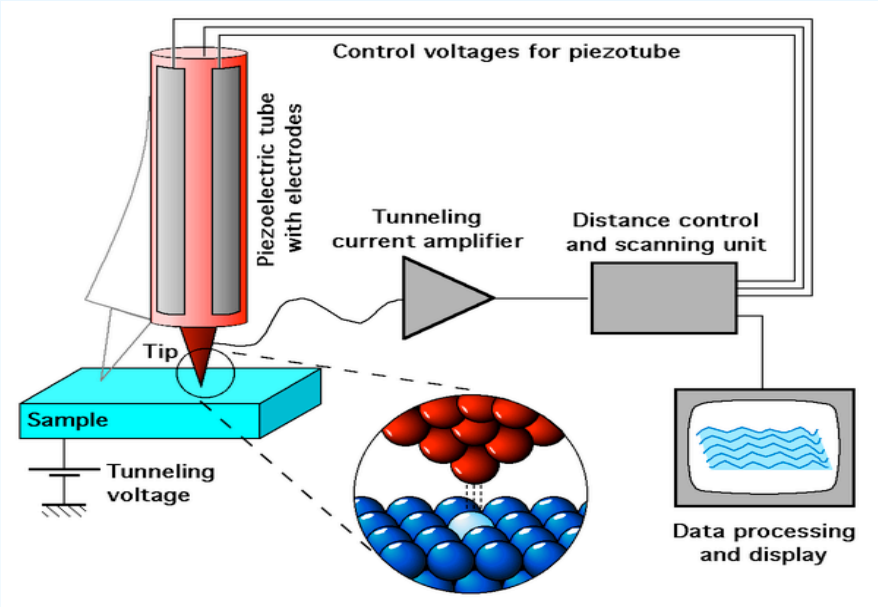
Neutrons are electrically neutral, they penetrate matter more deeply, provide valuable probes of bulk properties.

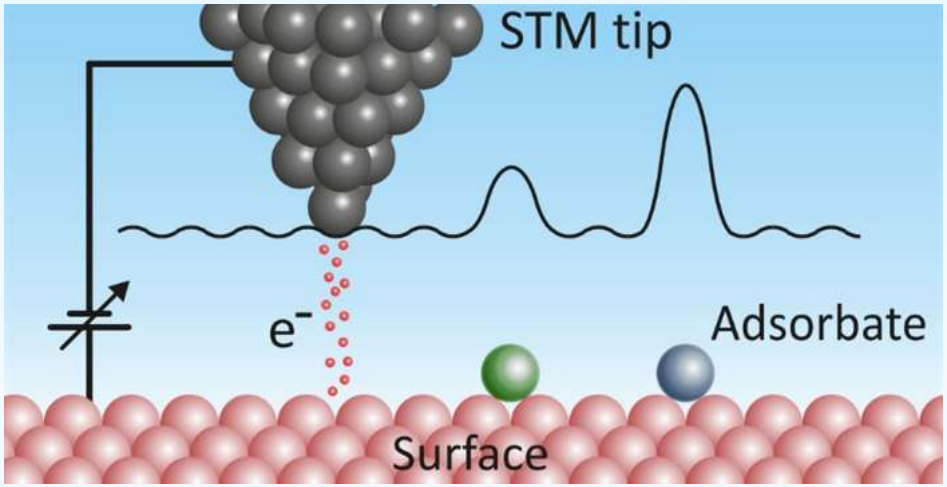
Neutrons carry spin, and thus can be used to detect magnetic periodic structure (long-range order).

Scanning tunneling microscope



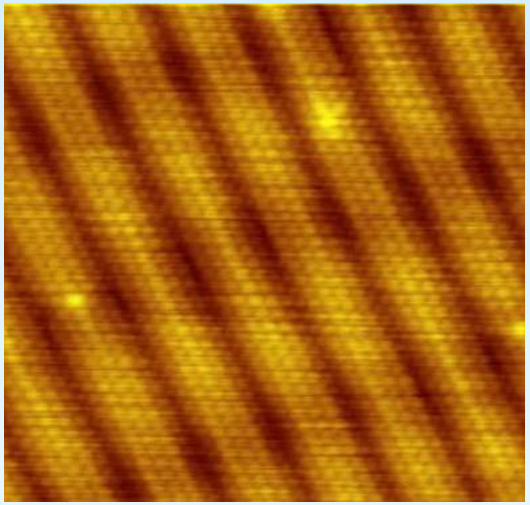




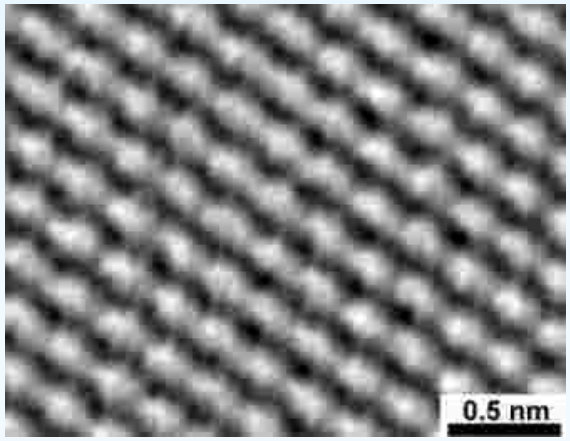


北京航空航天大學
BEIHANG UNIVERSITY

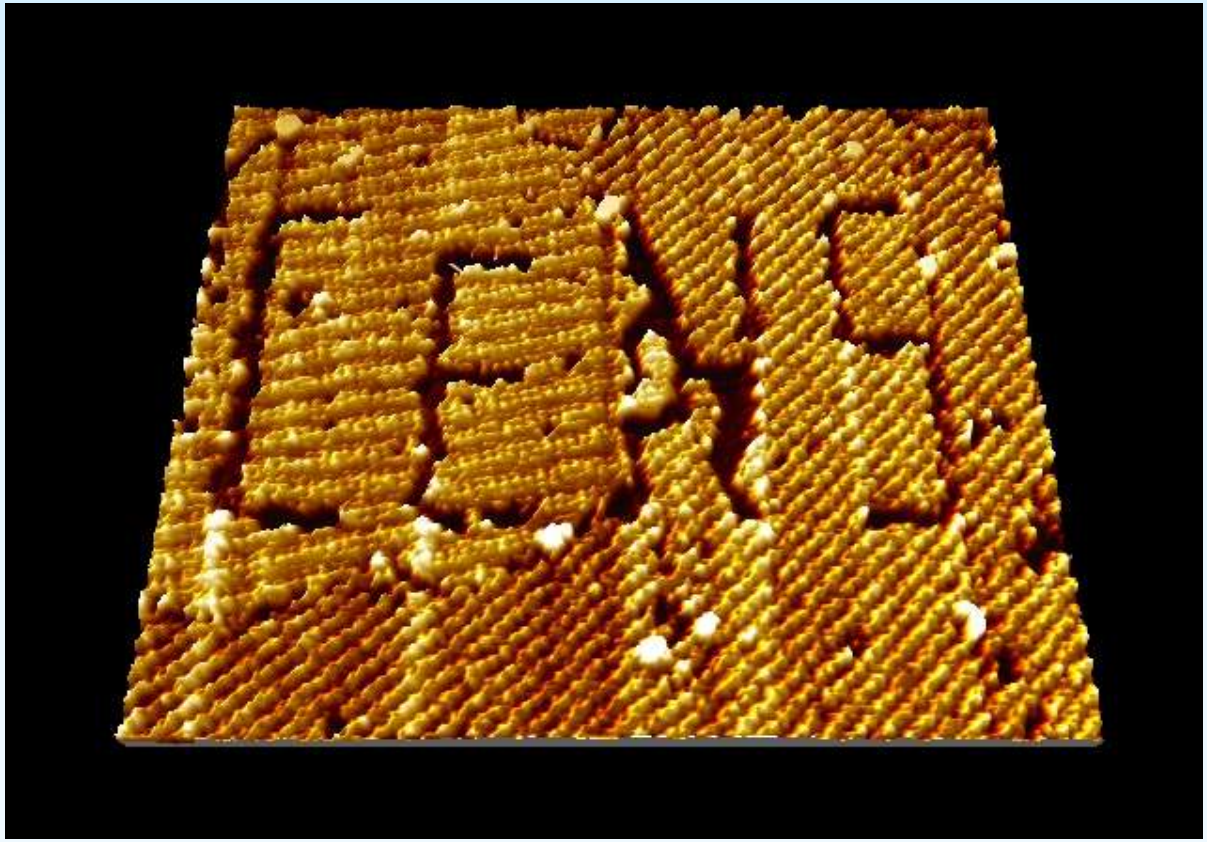
Scanning tunneling microscope



Gold 100 surface



Graphite surface



Nanomanipulation via STM of a self-assembled organic semiconductor monolayer (here: PTCDA molecules) on graphite, in which the logo of the Center for NanoScience (CeNS), LMU has been written

习题 XRD 分析

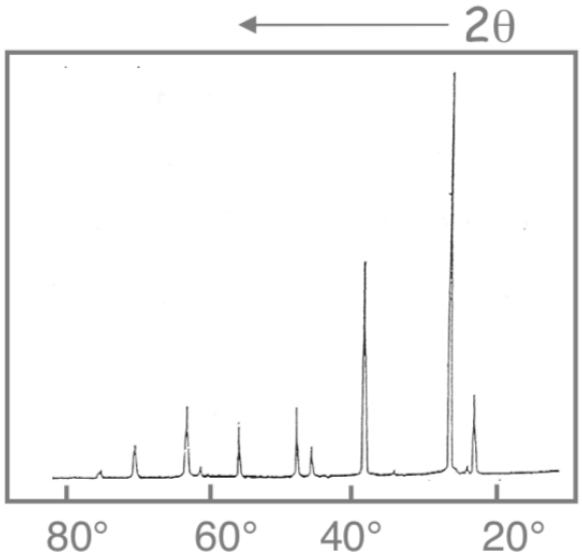
The powder method is used to record the diffraction patterns of cubic crystals : simple cubic, body-centerd cubic, face-centered cubic.

a) Recall how, using the Bragg relation, one can index the characteristic diffraction peaks of a cubic crystal and determine the lattice parameter.

b) Evaluate the structure factors of the different cubic structures and deduce in each case the allowed peaks.

c) Figure 3 drawn below represents the profile of the X-ray intensities diffracted by a cubic crystal (powder diagram). The measurement of the scattering angle for the two first peaks is 23°6 and 27°1. Determine the Bravais lattice of the corresponding crystal and index the observed peaks. Evaluate the lattice parameter, knowing that the radiation used is the K_α radiation of copper with a wavelength λ = 1,54Å.

Figure 3



The Bragg condition is :

$$2d_{hkl}\sin\theta = 2\frac{2\pi}{\left|\vec{G}_{hkl}\right|}\sin\theta = \lambda \Leftrightarrow \Delta\vec{s} = \vec{s} - \vec{s_0} = \vec{G}$$

où $\vec{G} = h\vec{A} + k\vec{B} + l\vec{C}$

For a simple cubic lattice of lattice parameter a, we have :

$$\left|\vec{A}\right| = \left|\vec{B}\right| = \left|\vec{C}\right| = \frac{2\pi}{a}, \quad \text{donc} \quad d_{hkl} = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$$

and the Bragg relation is written as:

$$2\frac{a}{\sqrt{h^2 + k^2 + l^2}}\sin\theta = \lambda$$

In the powder method, the Bragg reflection for a given angle θ is associated to a set of equivalent planes as for example :

$$(111), (\bar{1}11), (11\bar{1}), (1\bar{1}1), (\bar{1}\bar{1}1), (\bar{1}1\bar{1}), (\bar{1}\bar{1}\bar{1})$$

The increasing values of θ (and so of $\sin\theta$) are associated with increasing values of $h^2 + k^2 + l^2$, with $\sin\theta \leq 1$. The first allowed reflections for a cubic lattice are:

$h^2 + k^2 + l^2$	h, k, l
1	100
2	110
3	111
4	200
5	210
6	211
8	220
9	300,221
10	310
11	311
12	222
13	320
14	321
16	400
17	410,322
18	411,330
19	331
20	420
21	421

$$F_{hkl} = \sum_i f_i e^{-i2\pi(hx_i + ky_i + lz_i)}$$

✓ consider the geometric structure factor

Simple cubic	Body centered cubic	Face centered cubic
100		
110	110	
111		111
200	200	200
210		
211	211	
220	220	220
300,221		
310	310	
311		311
222	222	222
320		
321	321	
400	400	400
410,322		
411,330	411,330	
331		331
420	420	420
421		

The corresponding angles of the diffraction reflected beams are given by:

$$\sin(\theta_{hkl}) = \frac{\lambda}{2a}\sqrt{h^2 + l^2 + k^2}$$

For the ratios of the 2 first angles, we obtain:

Simple cubic $\quad \frac{\sin\theta_{110}}{\sin\theta_{100}} = \sqrt{2} = 1.414$

Centered cubic $\quad \frac{\sin\theta_{200}}{\sin\theta_{110}} = \frac{2}{\sqrt{2}} = 1.414$

Face centered cubic $\quad \frac{\sin\theta_{200}}{\sin\theta_{111}} = \frac{2}{\sqrt{3}} = 1.154$

For our experimental spectrum:

$2\theta_1 = 23.6° \quad \theta_1 = 11.8° \quad \sin(11.8) = 0.2045$

$2\theta_2 = 27.1° \quad \theta_1 = 13.55° \quad \sin(13.55) = 0.2343$

So $\frac{\sin\theta_2}{\sin\theta_1} = \frac{0.2343}{0.2045} = 1.146$, the value corresponds to the face centered cubic lattice.

The allowed reflections are :
(111),(200),(220),(311),(222),(400),....

The lattice parameter is given by:

$$a = \frac{\lambda}{2\sin\theta_{hkl}}\sqrt{h^2 + k^2 + l^2}$$

$$a = 1.54\sqrt{3}\,\frac{1}{2 * 0.2045} = 6.52\ A$$