x-ray diffraction

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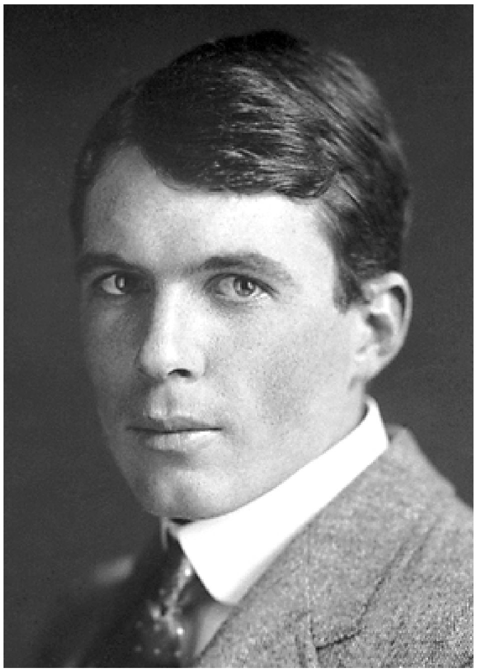
((William Lawrence Bragg))



Sir William Lawrence Bragg, (31 March 1890 – 1 July 1971) was an Australian-born British physicist and X-ray crystallographer, discoverer (1912) of Bragg's law of X-ray diffraction, which is basic for the determination of crystal structure. He was joint winner (with his father, William Henry Bragg) of the Nobel Prize in Physics in 1915: *"For their services in the analysis of crystal structure by means of X-ray"*, an important step in the development of X-ray crystallography. Bragg was knighted in 1941. As of 2018, he is the youngest ever Nobel laureate in physics, having received the award at the age of 25 years. Bragg was the director of the Cavendish Laboratory, Cambridge, when the discovery of the structure of DNA was reported by James D. Watson and Francis Crick in February 1953.
https://en.wikipedia.org/wiki/Lawrence_Bragg

Here we discuss the Bragg's law in the x-ray diffraction of crystals with periodicity. The construction of the Ewald sphere is useful for our understanding of the Bragg's law.

1. Introduction

1.1 x-ray source

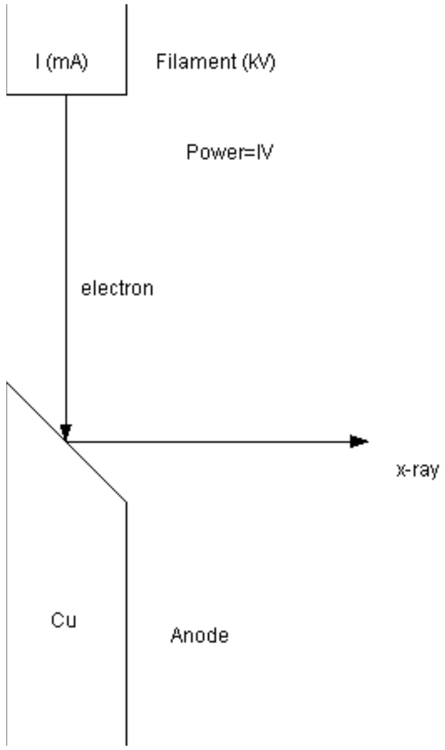


Fig. Schematic diagram for the generation of x-rays. Metal target (Cu or Mo) is bombarded by accelerating electrons. The power of the system is given by $P = I(\text{mA})\ V(\text{keV})$, where I is the current of cathode and V is the voltage between the anode and cathode. Typically, we have $I = 30$ mA and $V = 50$ kV: $P = 1.5$ kW.

We use two kinds of targets to generate x-rays: Cu and Mo.
The wavelength of $\text{CuK}_{\alpha 1}$, $\text{CuK}_{\alpha 2}$ and CuK_{β} lines are given by

$$\lambda_{K\alpha 1} = 1.540562\ \text{Å}. \quad \lambda_{K\alpha 2} = 1.544390\ \text{Å},\ \lambda_{K\beta} = 1.392218\ \text{Å}.$$

The intensity ratio of $\text{CuK}_{\alpha 1}$ and $\text{CuK}_{\alpha 2}$ lines is 2:1. The weighed average wavelength $\lambda_{K\alpha}$ is calculated as

$$\lambda_{K\alpha} = \frac{2\lambda_{K\alpha 1} + \lambda_{K\alpha 2}}{3} = 1.54184\ \text{Å}.$$

((**Note**)) The wavelength of MoKα is $\lambda_{K\alpha} = 0.71073$ Å. Figure shows the intensity versus wavelength distribution for x rays from a Mo target. The penetration depth of MoK_{α} line is much longer than that of CuK_{α} line.

$\lambda_{K\alpha 1} = 0.709300$ Å. $\lambda_{K\alpha 2} = 0.713590$ Å, $\lambda_{K\beta} = 0.632$ Å

$$\lambda_{K\alpha} = \frac{2\lambda_{K\alpha 1} + \lambda_{K\alpha 2}}{3} = 0.71073 \text{ Å}.$$

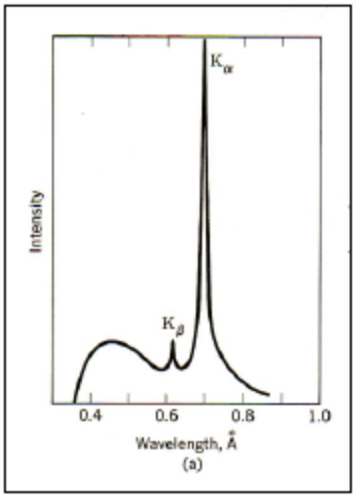
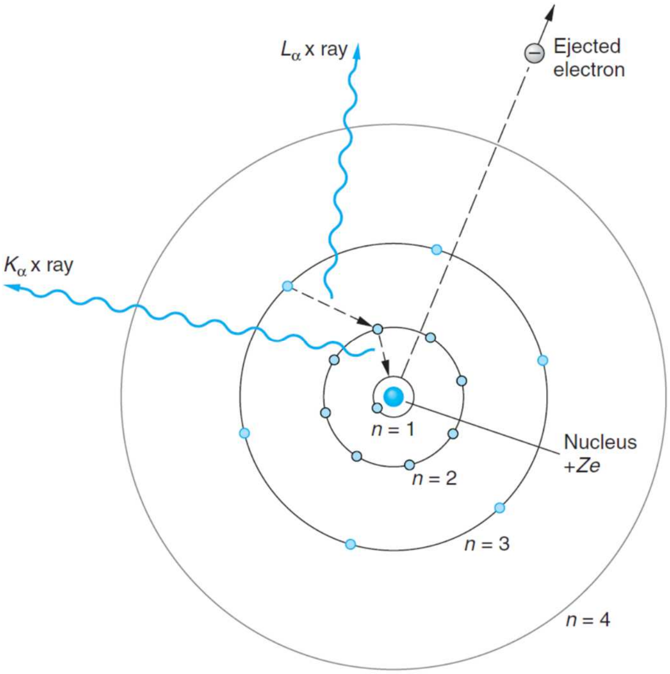


Fig. Intensitry vs wavelength distribution for x-rays from a Mo target bombarded by 30 keV electrons from C. Kittel, Introduction to Solid State Physics.



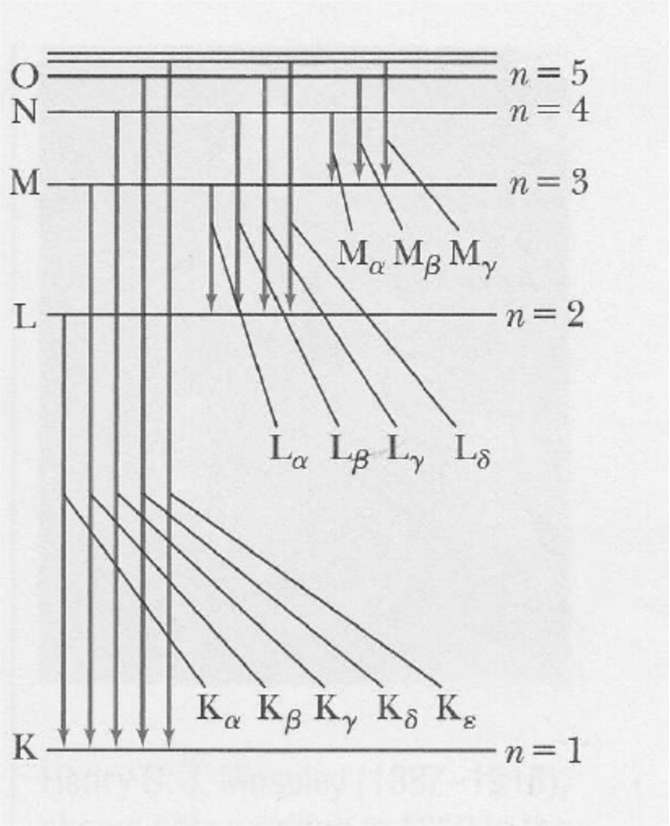


Fig. x-ray spectrum. K_α line (from $n = 2$ to $n = 1$). K_β line (from $n = 3$ to $n = 1$). and L_α line (from $n = 3$ to $n = 1$). n is the principal quantum number.

((**Example**)) Mo

Atomic number: $Z = 42$
proton 42, neutron 54
Atomic mass = 95.94 u

((**Formula**))

$$\frac{1}{\lambda(K_\alpha)} = R(Z-1)^2\left(\frac{1}{1^2}-\frac{1}{2^2}\right) = \frac{3}{4}R(Z-1)^2$$

with

$R = 1.0973731568539(55) \times 10^7$/m

(a)

$$\lambda(K_\alpha) = 0.0722798 \text{ nm} = 0.722798 \text{ Å}$$

(b)

$$\frac{1}{\lambda(K_\beta)} = R(Z-1)^2(\frac{1}{1^2} - \frac{1}{3^2}) = \frac{8}{9}R(Z-1)^2$$

$$\lambda(K_\beta) = 0.060986 \text{ nm} = 0.60986 \text{ Å}$$

$$\frac{1}{\lambda(K_\gamma)} = R(Z-1)^2(\frac{1}{1^2} - \frac{1}{4^2}) = \frac{15}{16}R(Z-1)^2$$

$$\lambda(K_\gamma) = 0.0578238 \text{ nm} = 0.578238 \text{ Å}$$

$$\frac{1}{\lambda(K_\infty)} = R(Z-1)^2(\frac{1}{1^2} - \frac{1}{\infty^2}) = R(Z-1)^2$$

$$\lambda(K_\infty) = 0.0542098 \text{ nm} = 0.542098 \text{ Å}$$

Link:
http://www.xtal.iqfr.csic.es/Cristalografia/parte_02-en.html

1.2 Principle of x-ray diffraction

x-ray (photon) behaves like both wave and particle. In a crystal, atoms are periodically located on the lattice. Each atom has a nucleus and electrons surrounding the nucleus. The electric field of the incident photon accelerates electrons. The electrons oscillate around an equilibrium position with the period of the incident photon. The nucleus does not oscillate because of the heavy mass.

Classical electrodynamics tells us that an accelerating charge radiates an electromagnetic field.

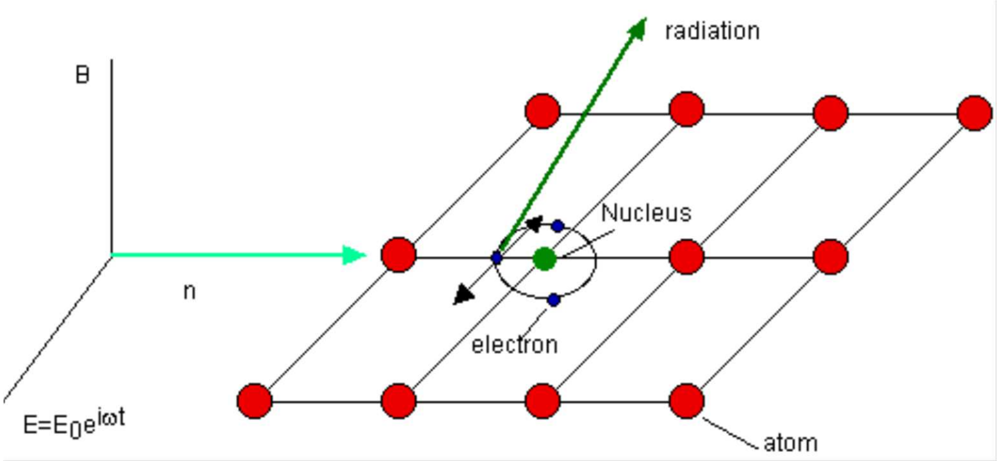


Fig. Schematic diagram for the interaction between an electromagnetic wave (x-ray) and electrons surrounding nucleus. The oscillatory electric field ($E = E_0e^{i\omega t}$) of x-ray photon gives rise to the harmonic oscillation of the electrons along the electric field.

The instantaneous electromagnetic energy (radiation) flow is given by the pointing vector

$$\boldsymbol{S} \approx \frac{\dot{v}^2 \sin^2\theta}{R^2}\boldsymbol{n}.$$

The direction of the velocity $\boldsymbol{v}$ (the direction of the oscillation) is along the x direction. The direction of the photon radiation is in the (x, y) plane.

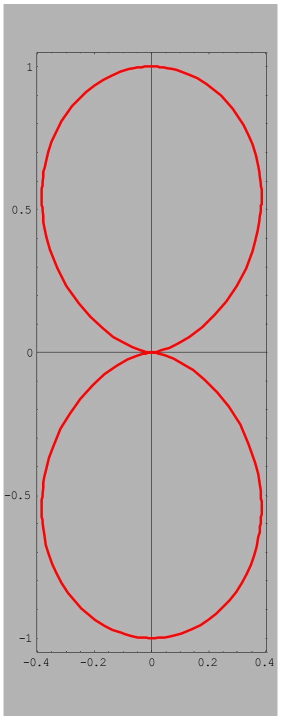


Fig. The distribution of instantaneous radiation energy due to the oscillation of electrons along the *x* direction.

1.3 Experimental configuration of x-ray scattering

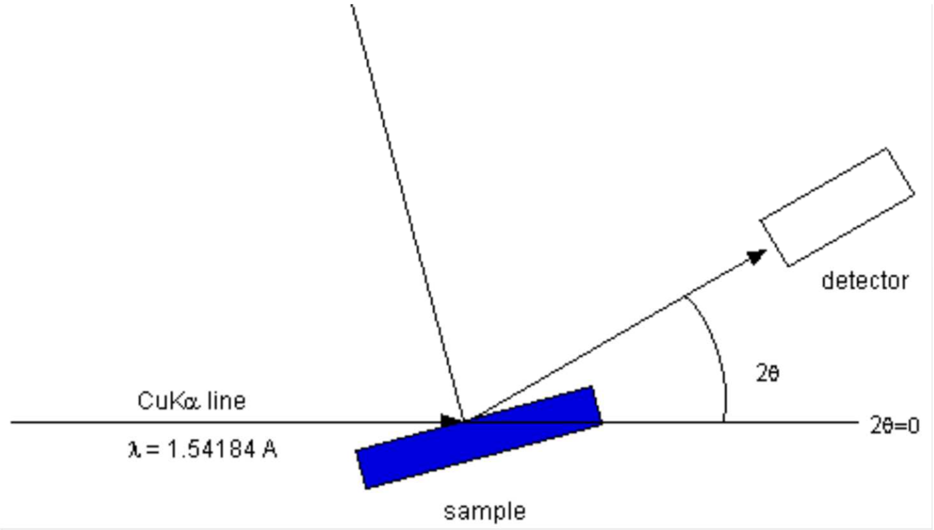


Fig. Example for the geometry of Ω (= θ) – 2θ scan for the (00*L*) x-ray diffraction. The Cu target is used. The direction of the incident x-ray is $2\theta = 0$. The angle between the detector and the direction of the incident x-ray is 2θ. W is the rotation angle of the sample.

((**Example**)) x-ray diffraction

We show two examples of the x-ray diffraction pattern whicha are obtained in my laboratory

(a) Stage- 3 $MoCl_5$ graphite intercalation compound (GIC). $MoCl_5$ are intercalated into empty graphite galleries. There are three graphene layers between adjacent MoCl5 intercalate layers.

(b) Ni vemiculite. Vermiculite is a layered silicate (a kind of clays). In the interlamellar space, Ni layer are sandwiched between two water layers.

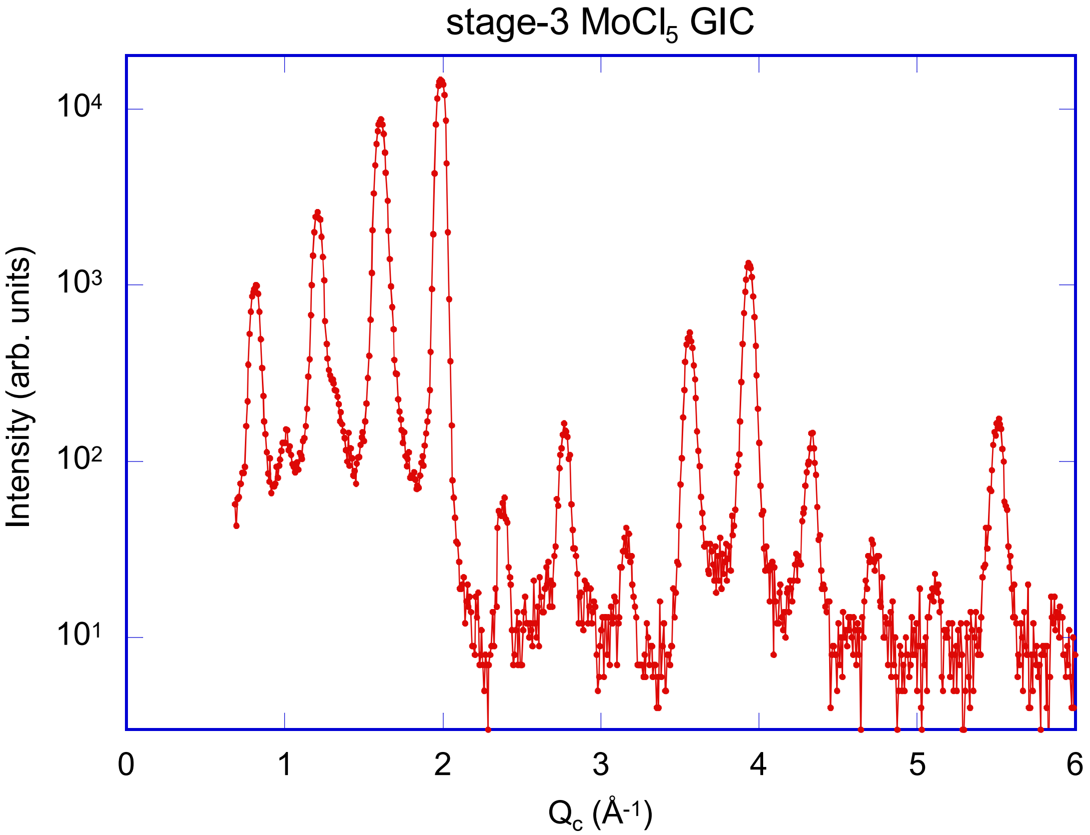


Fig. (00*L*) x-ray diffraction pattern of stage-3 $MoCl_5$ GIC (graphite intercalation compound)

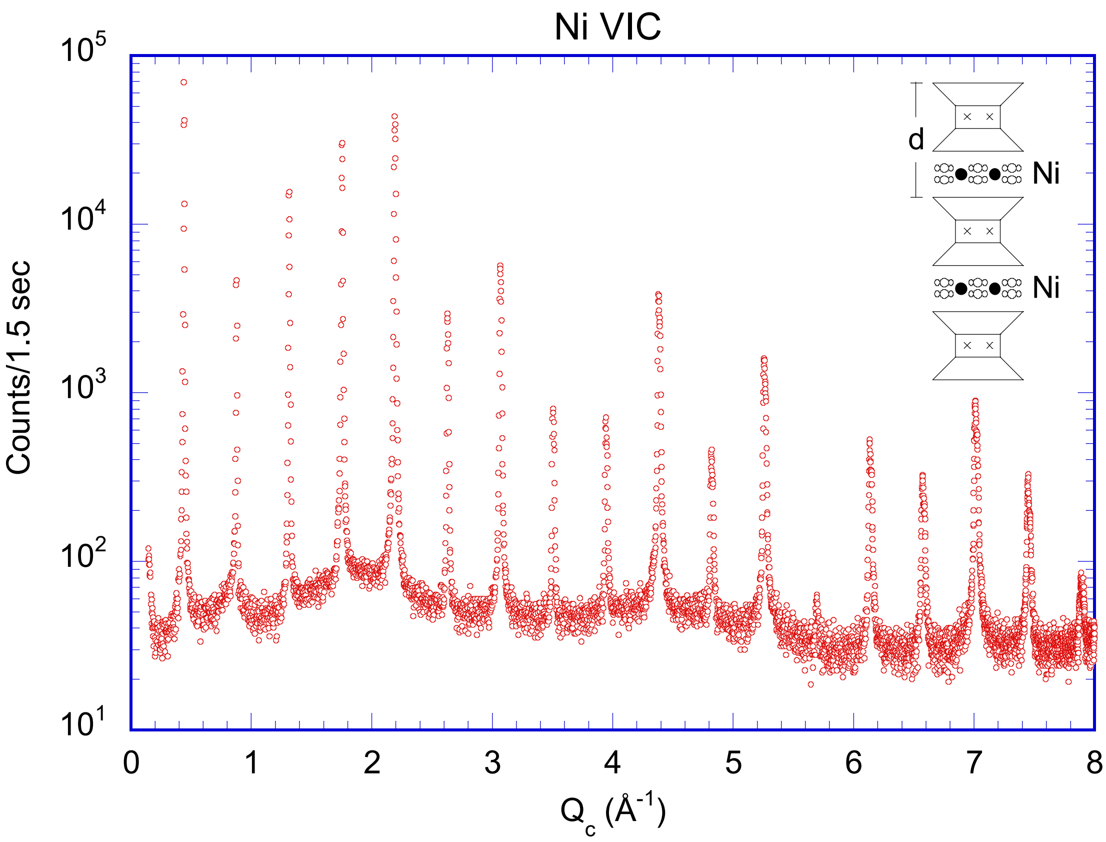


Fig. (00*L*) x-ray diffraction pattern of Ni-vermiculite with two water-layer hydration state.

2 Born approximation in quantum mechanics

2.1 Green's function in scattering theory

We start with the original Schrödinger equation.

$$-\frac{\hbar^2}{2\mu}\nabla^2\psi(\boldsymbol{r})+V(\boldsymbol{r})\psi(\boldsymbol{r})=E_k\psi(\boldsymbol{r}),$$

or

$$(\nabla^2+\frac{2\mu}{\hbar^2}E_k)\psi(\boldsymbol{r})=\frac{2\mu}{\hbar^2}V(\boldsymbol{r})\psi(\boldsymbol{r}).$$

under the potential energy $V(\boldsymbol{r})$. We assume that

$$E=E_k=\frac{\hbar^2}{2\mu}k^2,$$

We put

$$f(\boldsymbol{r}) = -\frac{2\mu}{\hbar^2} V(\boldsymbol{r})\psi(\boldsymbol{r}),$$

Using the operator

$$L_{\mathbf{r}} = \nabla^2 + k^2.$$

we have the differential equation

$$L_r \psi(\boldsymbol{r}) = (\nabla^2 + k^2)\psi(\boldsymbol{r}) = -f(\boldsymbol{r}).$$

Suppose that there exists a Green's function $G(\boldsymbol{r})$ such that

$$(\nabla_r{}^2 + k^2)G^{(+)}(\boldsymbol{r},\boldsymbol{r}') = -\delta(\boldsymbol{r}-\boldsymbol{r}'),$$

with

$$G^{(+)}(\boldsymbol{r},\boldsymbol{r}') = \frac{\exp(ik|\boldsymbol{r}-\boldsymbol{r}'|)}{4\pi|\boldsymbol{r}-\boldsymbol{r}'|} \qquad \text{(Green function)}$$

We will discuss about the derivation of this Green function later. Then $\psi(\mathbf{r})$ is formally given by

$$\begin{aligned}\psi^{(+)}(\boldsymbol{r}) &= \phi(\boldsymbol{r}) + \int d\boldsymbol{r}' G^{(+)}(\boldsymbol{r},\boldsymbol{r}') f(\boldsymbol{r}') \\ &= \phi(\boldsymbol{r}) - \frac{2\mu}{\hbar^2}\int d\boldsymbol{r}' \frac{\exp(ik|\boldsymbol{r}-\boldsymbol{r}'|)}{4\pi|\boldsymbol{r}-\boldsymbol{r}'|} V(\boldsymbol{r}')\psi^{(+)}(\boldsymbol{r}')\end{aligned},$$

where $\phi(\mathbf{r})$ is a solution of the homogeneous equation satisfying

$$(\nabla^2 + k^2)\phi(\boldsymbol{r}) = 0,$$

or

$$\phi(\boldsymbol{r}) = \langle \boldsymbol{r}|\boldsymbol{k}\rangle = \frac{1}{(2\pi)^{3/2}}\exp(i\boldsymbol{k}\cdot\boldsymbol{r}), \qquad \text{(plane wave)}$$

with

$$k = |\boldsymbol{k}|$$

Note that

$$
\begin{aligned}
(\nabla^2 + k^2)\psi(\boldsymbol{r}) &= (\nabla^2 + k^2)\phi(\boldsymbol{r}) + \int d\boldsymbol{r}'(\nabla^2 + k^2)G^{(+)}(\boldsymbol{r},\boldsymbol{r}')f(\boldsymbol{r}') \\
&= -\int d\boldsymbol{r}'\delta(\boldsymbol{r}-\boldsymbol{r}')f(\boldsymbol{r}') \\
&= -f(\boldsymbol{r})
\end{aligned}
$$

2.2 Born approximation

We start with

$$
\psi^{(+)}(\boldsymbol{r}) = \phi(\boldsymbol{r}) - \frac{2\mu}{\hbar^2}\int d\boldsymbol{r}'\frac{\exp(ik|\boldsymbol{r}-\boldsymbol{r}'|)}{4\pi|\boldsymbol{r}-\boldsymbol{r}'|}V(\boldsymbol{r}')\psi^{(+)}(\boldsymbol{r}'),
$$

$$
\phi(\boldsymbol{r}) = \langle r|\boldsymbol{k}\rangle = \frac{1}{(2\pi)^{3/2}}\exp(i\boldsymbol{k}\cdot\boldsymbol{r}), \qquad \text{(plane wave).}
$$

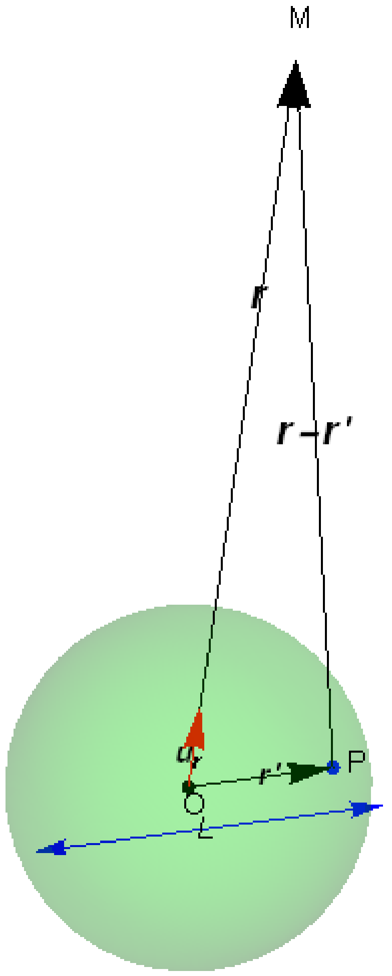


Fig. Vectors *r* and *r'* in calculation of scattering amplitude in the first Born approximation

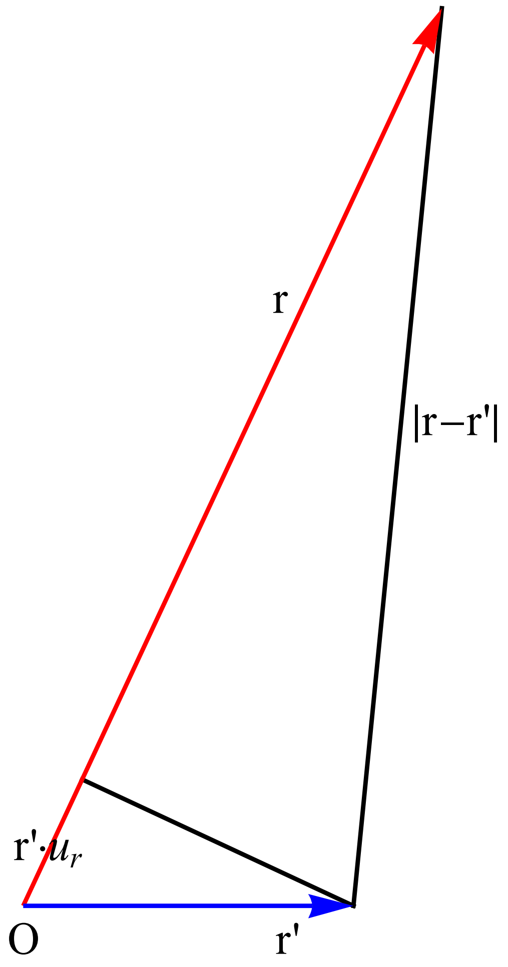


Fig. $\boldsymbol{u}_r = \boldsymbol{e}_r$

Here we consider the case of $\psi^{(+)}(r)$

$$|\boldsymbol{r}-\boldsymbol{r}'| \approx r - \boldsymbol{r}'\cdot\boldsymbol{e}_r$$

$$\boldsymbol{k}' = k\boldsymbol{e}_r$$

$$e^{ik|\boldsymbol{r}-\boldsymbol{r}'|} \approx e^{ik(r-\boldsymbol{r}'\cdot\boldsymbol{e}_r)} = e^{ikr}e^{-i\boldsymbol{k}'\cdot\boldsymbol{r}'}$$ for large *r*.

$$\frac{1}{|\boldsymbol{r}-\boldsymbol{r}'|} \approx \frac{1}{r}$$

Then we have

$$\psi^{(+)}(r) = \frac{1}{(2\pi)^{3/2}} \exp(i\boldsymbol{k}\cdot\boldsymbol{r}) - \frac{2\mu}{\hbar^2}\frac{1}{4\pi}\frac{e^{ikr}}{r}\int d\boldsymbol{r}' e^{-i\boldsymbol{k}'\cdot\boldsymbol{r}'} V(\boldsymbol{r}')\psi^{(+)}(\boldsymbol{r}')$$

or

$$\psi^{(+)}(r) = \frac{1}{(2\pi)^{3/2}}[e^{i\boldsymbol{k}\cdot\boldsymbol{r}} + \frac{e^{ikr}}{r} f(\boldsymbol{k}',\boldsymbol{k})]$$

The first term denotes the original plane wave in the propagation direction ***k***. The second term denotes the outgoing spherical wave with amplitude, $f(\boldsymbol{k}',\boldsymbol{k})$,

$$f(\boldsymbol{k}',\boldsymbol{k}) = -\frac{1}{4\pi}(2\pi)^{3/2}\frac{2\mu}{\hbar^2}\int d\boldsymbol{r}' e^{-i\boldsymbol{k}'\cdot\boldsymbol{r}'} V(\boldsymbol{r}')\psi^{(+)}(\boldsymbol{r}') .$$

The first Born approximation:

$$\begin{aligned} f(\boldsymbol{k}',\boldsymbol{k}) &= -\frac{1}{4\pi}\frac{2\mu}{\hbar^2}\int d\boldsymbol{r}' e^{-i\boldsymbol{k}'\cdot\boldsymbol{r}'} V(\boldsymbol{r}') e^{i\boldsymbol{k}\cdot\boldsymbol{r}'} \\ &= -\frac{\mu}{2\pi\hbar^2}\int d\boldsymbol{r}' V(\boldsymbol{r}') e^{-i(\boldsymbol{k}'-\boldsymbol{k})\cdot\boldsymbol{r}'} \end{aligned}$$

when $\psi^{(+)}(r)$ is approximated by

$$\psi^{(+)}(r) \approx \frac{1}{(2\pi)^{3/2}} e^{i\mathbf{k}\cdot\mathbf{r}} .$$

Note that $f(\boldsymbol{k}',\boldsymbol{k})$ is the Fourier transform of the potential energy with the wave vector ***Q***; the scattering vector;

$$\boldsymbol{Q} = \boldsymbol{k}' - \boldsymbol{k} .$$

Formally $f(\boldsymbol{k}',\boldsymbol{k})$ can be rewritten as

$$\begin{aligned} f(\boldsymbol{k}',\boldsymbol{k}) &= -\frac{\mu}{2\pi\hbar^2}(2\pi)^3 \langle \boldsymbol{k}'|\hat{V}|\boldsymbol{k}\rangle \\ &= -\frac{4\pi^2\mu}{\hbar^2}\langle \boldsymbol{k}'|\hat{V}|\boldsymbol{k}\rangle \end{aligned}$$

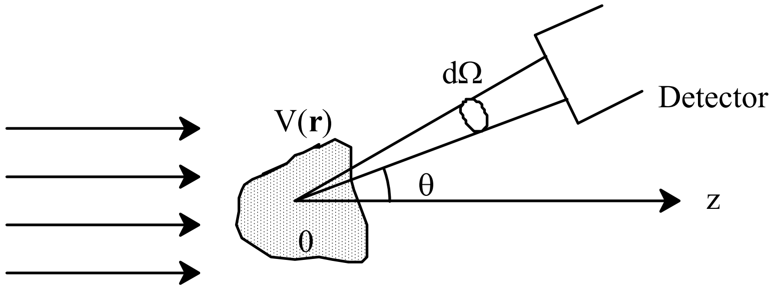
where

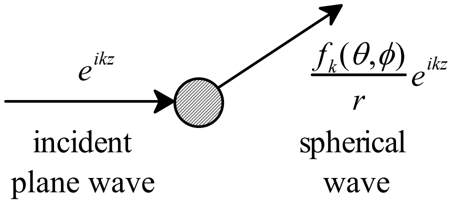
$$\langle \boldsymbol{k}'|\hat{V}|\boldsymbol{k}\rangle = \int d^3\boldsymbol{r}\langle \boldsymbol{k}'|\boldsymbol{r}\rangle V(\boldsymbol{r})\langle \boldsymbol{r}|\boldsymbol{k}\rangle$$
$$= \frac{1}{(2\pi)^3}\int d^3\boldsymbol{r} e^{-i(\boldsymbol{k}'-\boldsymbol{k})\cdot\boldsymbol{r}} V(\boldsymbol{r})$$

with

$$\langle \boldsymbol{r}|\boldsymbol{k}\rangle = \frac{1}{(2\pi)^{3/2}}\exp(i\boldsymbol{k}\cdot\boldsymbol{r})$$

2.3 Differential cross section





We define the differential cross section $\frac{d\sigma}{d\Omega}$ as the number of particles per unit time scattered into an element of solid angle $d\Omega$ divided by the incident flux of particles.

The probability flux associated with a wave function

$$\phi_k(\boldsymbol{r}) = \langle \boldsymbol{r}|\boldsymbol{k}\rangle = \frac{1}{(2\pi)^{3/2}}e^{i\boldsymbol{k}\cdot\boldsymbol{r}} = \frac{1}{(2\pi)^{3/2}}e^{ikz},$$

is obtained as

$$N_z = J_z = \frac{\hbar}{2\mu i}[\phi_k^*(\boldsymbol{r})\frac{\partial}{\partial z}\phi_k(\boldsymbol{r}) - \phi_k(\boldsymbol{r})\frac{\partial}{\partial z}\phi_k^*(\boldsymbol{r})] = \frac{1}{(2\pi)^3}\frac{\hbar k}{\mu} = \frac{v}{(2\pi)^3}$$

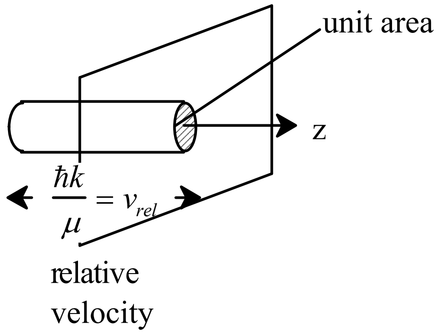


Fig.

$$\text{volume} = \frac{\hbar k}{\mu} \times 1$$

$\left| e^{ikz} \right|^2 = 1$ means that there is one particle per unit volume. J_z is the probability flow (probability per unit area per unit time) of the incident beam crossing a unit surface perpendicular to OZ

The probability flux associated with the scattered wave function

$$\chi_r = \frac{1}{(2\pi)^{3/2}} \frac{e^{ikr}}{r} f(\theta) \qquad \text{(spherical wave)}$$

is

$$J_r = \frac{\hbar}{2\mu i}(\chi_r^* \frac{\partial}{\partial r}\chi_r - \chi_r \frac{\partial}{\partial r}\chi_r^*) = \frac{1}{(2\pi)^3} \frac{\hbar k}{\mu} \frac{|f(\theta)|^2}{r^2}$$

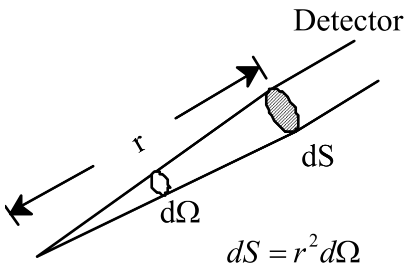
Since

$$dA = r^2 d\Omega$$

we have

$$\Delta N = J_r dA = \frac{v}{(2\pi)^3} \frac{|f(\theta)|^2}{r^2} r^2 d\Omega = \frac{v}{(2\pi)^3} |f(\theta)|^2 d\Omega$$

where J_r is the probability flow (probability per unit area per unit time)



The differential cross section

$$\frac{d\sigma}{d\Omega} d\Omega = \frac{\Delta N}{N_z} = \left| f(\theta) \right|^2 d\Omega$$

or

$$\frac{\partial \sigma}{\partial \Omega} = \left| f(\theta) \right|^2 .$$

First-order Born amplitude:

$$\begin{aligned} f(\boldsymbol{k}', \boldsymbol{k}) &= -\frac{1}{4\pi} (2\pi)^3 \frac{2\mu}{\hbar^2} \langle \boldsymbol{k}' | V | \boldsymbol{k} \rangle \\ &= -\frac{\mu}{2\pi\hbar^2} \int d^3\boldsymbol{r}' e^{-i(\boldsymbol{k}'-\boldsymbol{k})\cdot\boldsymbol{r}} V(\boldsymbol{r}') , \\ &= -\frac{\mu}{2\pi\hbar^2} \int d^3\boldsymbol{r}' e^{-i\boldsymbol{Q}\cdot\boldsymbol{r}} V(\boldsymbol{r}') \end{aligned}$$

which is the Fourier transform of the potential with respect to $\boldsymbol{Q}$, where

$\boldsymbol{Q} = \boldsymbol{k}' - \boldsymbol{k}$: scattering wave vector.

$|\boldsymbol{Q}| = Q = 2k \sin\theta$ for the elastic scattering.

The Ewald sphere is given by this figure. In the case of x-ray and neutron diffraction, we use the scattering angle 2θ, instead of θ.

((Ewald sphere)) x-ray and neutron scattering

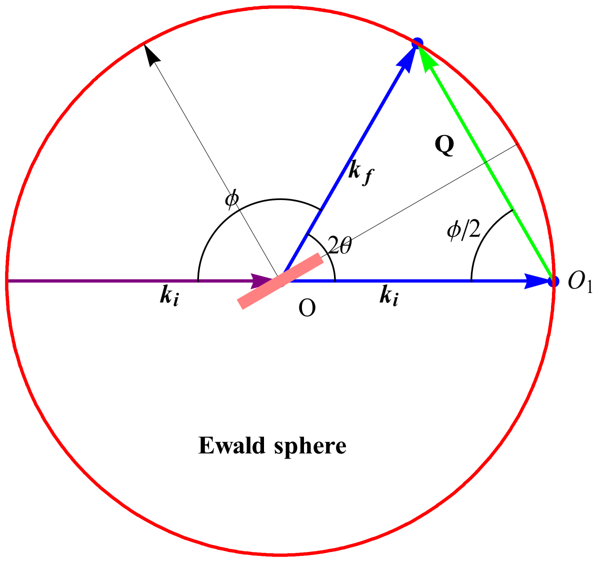


Fig. Ewald sphere used for the x-ray and neutron scattering experiments. $\boldsymbol{k}_{\mathrm{i}} = \boldsymbol{k}$. $\boldsymbol{k}_{\mathrm{f}} = \boldsymbol{k}'$. $\boldsymbol{Q} = \boldsymbol{q} = \boldsymbol{k} - \boldsymbol{k}'$ (scattering wave vector). Note that in the conventional x-ray and neutron scattering experiments, we use the angle 2θ, instead of θ for both the x-ray and neutron scattering,

3. Bragg condition

3.1. Bragg law

The incident x-rays are reflected specularly from parallel planes of atoms in the crystal.

(a) The angle of incoming x-rays is equal to the angle of outgoing x-rays.

(b) The energy of x-rays is conserved on reflection (elastic scattering).

The path difference for x-rays reflected from adjacent planes is equal to $\Delta d = 2d \sin\theta$. The corresponding phase difference is

$$\Delta\phi = k\Delta d = (2\pi/\lambda)2d \sin\theta .$$

where k is the wave number ($k = 2\pi/\lambda$) and λ is the wave length.

Constructive interference of the radiation from successive planes occurs when $\Delta\phi = 2n\pi$, where n is an integer (Bragg's law).

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

The Bragg reflection can occur only for $\lambda \leq 2d$.

The Bragg law is a consequence of the periodicity of the lattice. The Bragg law does not refer to the composition of the basis of atoms associated with every lattice point. The composition of the bases determines the relative intensity of the various orders of diffraction.

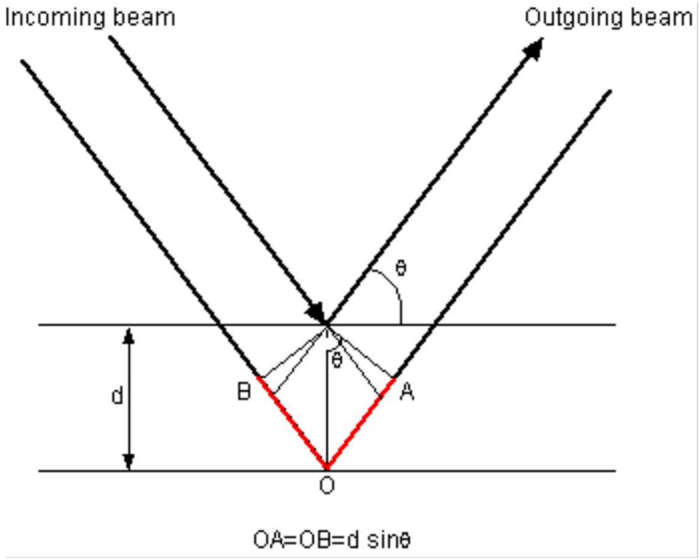
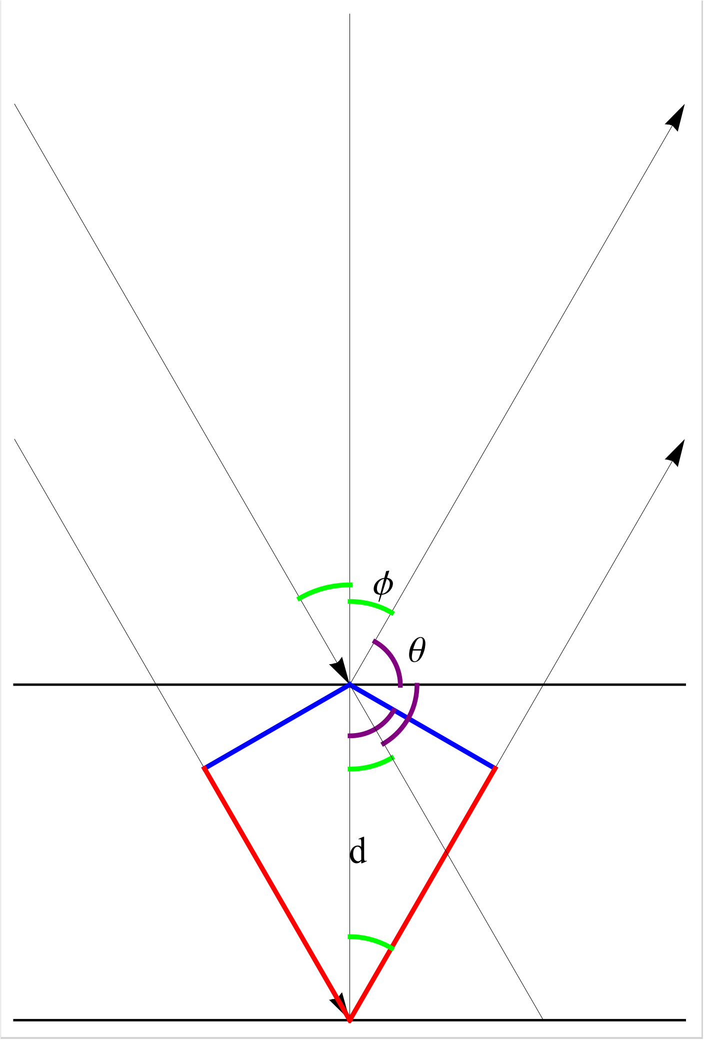
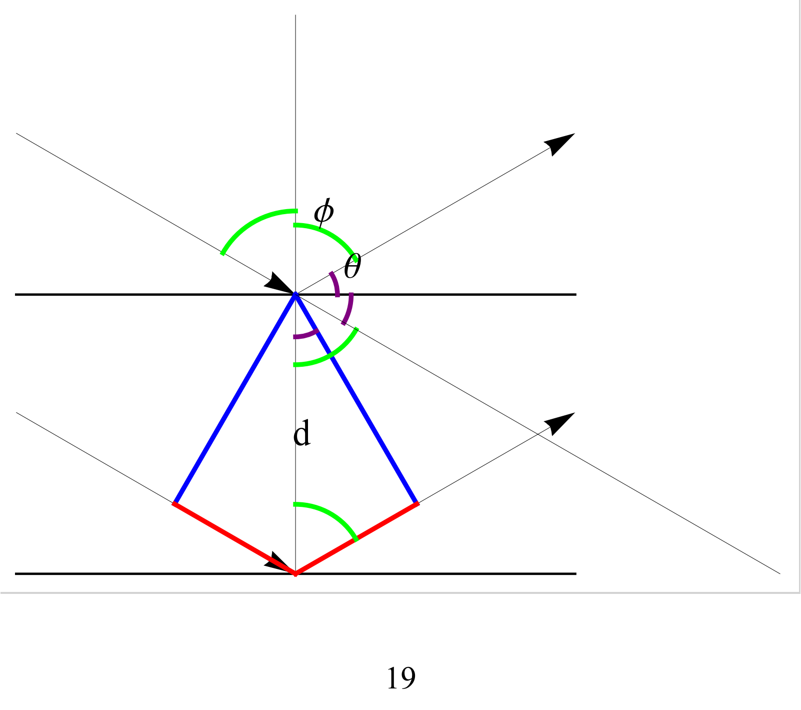


Fig. Geometry of the scattering of x-rays from planar arrays. The path difference between two rays reflected by planar arrays is $2d\sin\theta$.



ϕ
θ
d



ϕ
θ
d

Fig. Path of ray-1 and ray-2; $\theta + \phi = \frac{\pi}{2}$. The path difference is denoted by the red line. The Bragg law is satisfied by $2d\sin\theta = l\lambda$.

3.2 Concept of Ewald sphere: introduction of reciprocal lattice

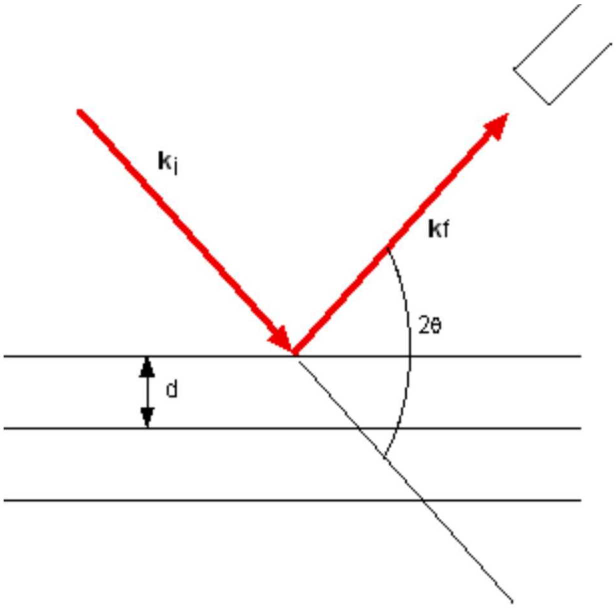


Fig. The geometry of the scattered x-ray beam. The incident x-ray has the wavevector k_i (= $\boldsymbol{k}$), while the outgoing x-ray has the wavevector $\boldsymbol{k}_f$ (= $\boldsymbol{k}'$). $|\boldsymbol{k}_i| = |\boldsymbol{k}_f| = 2\pi/\lambda$, where λ is the wavelength of x-ray.

Bragg law:

$$2d\sin\theta = l\lambda,$$

where $\boldsymbol{k}_i$ is incident wavevector, and $\boldsymbol{k}_f$ is the outgoing wavevector,

$$|\boldsymbol{k}_i| = |\boldsymbol{k}_f| = \frac{2\pi}{\lambda}.$$

$\boldsymbol{Q}$ is the scattering vector:

$$\boldsymbol{Q} = \boldsymbol{k}_i - \boldsymbol{k}_f, \quad \text{or} \quad \boldsymbol{Q} = \boldsymbol{k}_f - \boldsymbol{k}_i$$

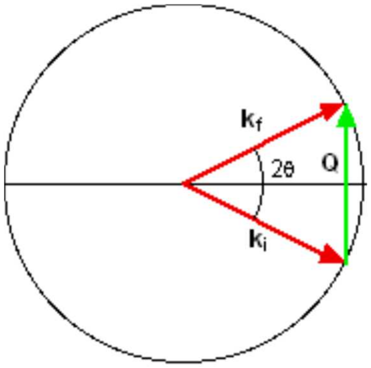


Fig. The geometry of Fig.10 using a circle with a radius k (= $2\pi/\lambda$). The scattering vector $\boldsymbol{Q}$ is defined by $\boldsymbol{Q} = \boldsymbol{k}_f - \boldsymbol{k}_i$.

In the above configuration, $\boldsymbol{Q}$ is perpendicular to the surface of the system

$$|\boldsymbol{Q}| = 2|\boldsymbol{k}_i|\sin\theta = \frac{4\pi}{\lambda}\sin\theta = \frac{4\pi}{\lambda}\frac{n\lambda}{2d} = \frac{2\pi}{d}n \text{ (Bragg condition).}$$

which coincides with the reciprocal lattice point. In other words, the Bragg reflections occur, when $\boldsymbol{Q}$ is equal to the reciprocal lattice vectors $\boldsymbol{G}$.

The Ewald sphere (shown below) is essential to understanding the above concept. The Bragg law means that the Bragg reflection occurs when the scattering vector Q coincides with the reciprocal lattice vector;

$$\boldsymbol{Q} = \boldsymbol{k}_f - \boldsymbol{k}_i = \boldsymbol{G}$$

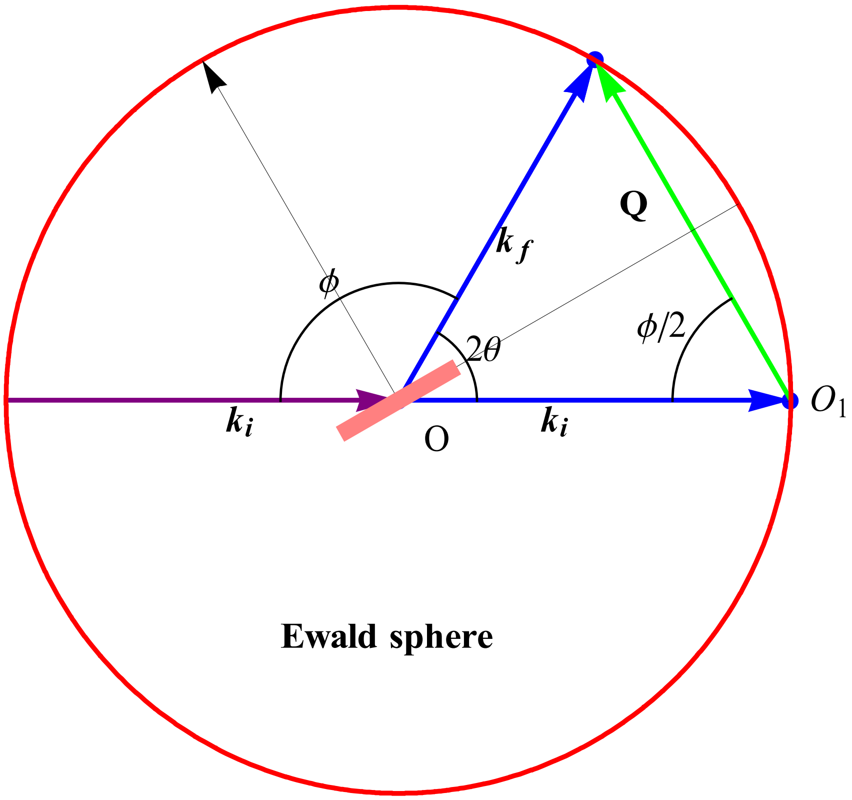


Fig. **Ewald sphere**. k_i ($|k_i| = 2\pi/\lambda$) is the wave vector of the incoming x-ray. k_f is the wave vector of the outgoing x-xay. The scattering vector $\boldsymbol{Q}$ (= $\boldsymbol{G}$) is parallel to the c axis of the sample located on the origin O. $|\boldsymbol{Q}| = (4\pi/\lambda)\sin\theta$. O1 is the origin of the reciprocal lattice space of the sample.

4. 1D reciprocal lattice

We consider a linear chain with a lattice constant $a_1 = a$ (a primitive cell). The corresponding reciprocal lattice is formed of a 1D reciprocal lattice with a reciprocal lattice constant b_1 ($=2\pi/a_1$), where

$$a_1 \cdot b_1 = 2\pi .$$

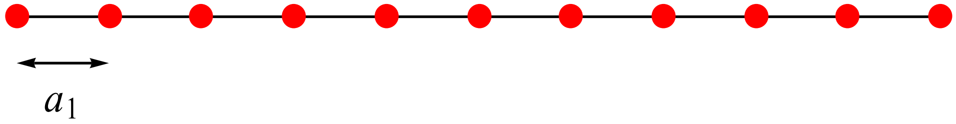


Fig. 1 D lattice with a lattice constant a_1.

Fig. 1D reciprocal lattice with a reciprocal lattice b_1 (= $2\pi/a_1$)

5 2D Reciprocal lattice vector

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

5.1 Square lattice

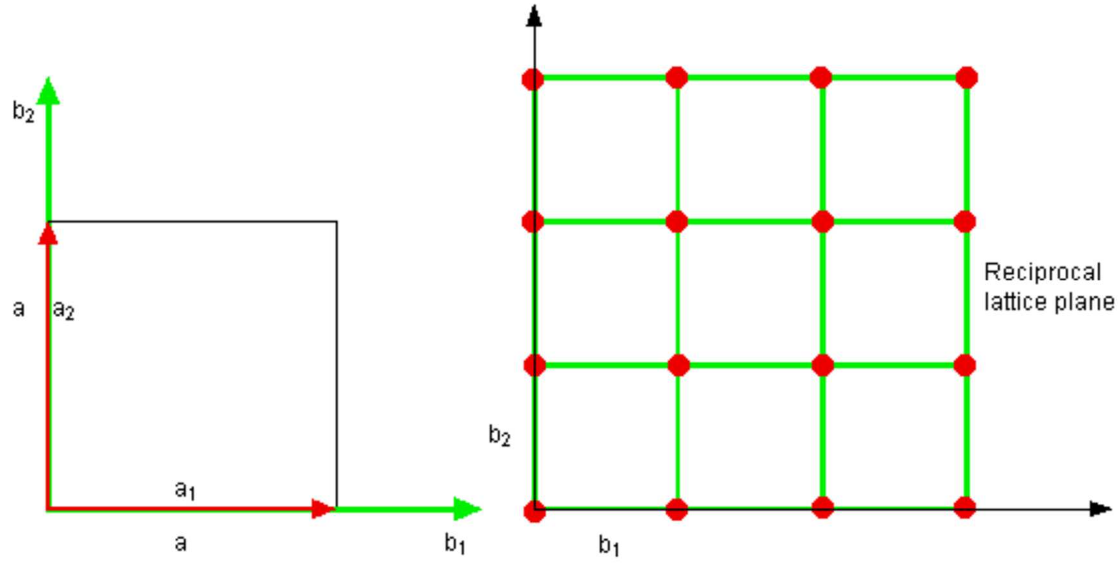


Fig. Real space for the square lattice and the corresponding reciprocal lattice plane.

$\boldsymbol{a}_1$ and $\boldsymbol{a}_2$ are the lattice vectors, and $\boldsymbol{b}_1$ and $\boldsymbol{b}_2$ are the reciprocal lattice vectors. The direction of $\boldsymbol{b}_1$ ($\boldsymbol{b}_2$) is the same as that of $\boldsymbol{a}_1$ ($\boldsymbol{a}_2$).

$$\boldsymbol{a}_1 \cdot \boldsymbol{b}_1 = \boldsymbol{a}_2 \cdot \boldsymbol{b}_2 = 2\pi \quad \text{(inner product),} \qquad \boldsymbol{a}_1 \cdot \boldsymbol{b}_2 = \boldsymbol{a}_1 \cdot \boldsymbol{b}_2 = 0$$

$$a_1 b_1 = 2\pi \,, \qquad \text{or} \qquad b_1 = \frac{2\pi}{a_1}$$

$$a_2 b_2 = 2\pi \,, \qquad \text{or} \qquad b_2 = \frac{2\pi}{a_2}$$

5.2 Hexagonal lattice (or triangular lattice)

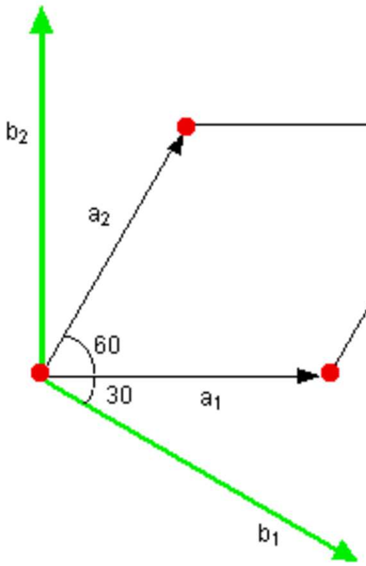


Fig. Real space for the hexagonal (triangular) lattice and the corresponding reciprocal lattice plane.

$\boldsymbol{a}_2$ is perpendicular to $\boldsymbol{b}_1$. $\boldsymbol{a}_1$ is perpendicular to $\boldsymbol{b}_2$.

$$\boldsymbol{a}_1 \cdot \boldsymbol{b}_1 = \boldsymbol{a}_2 \cdot \boldsymbol{b}_2 = 2\pi\ , \qquad \boldsymbol{a}_1 \cdot \boldsymbol{b}_2 = \boldsymbol{a}_1 \cdot \boldsymbol{b}_2 = 0$$

$$a_1 b_1 \cos(30^\circ) = 2\pi, \quad \text{or} \quad b_1 = \frac{4\pi}{\sqrt{3}a_1}$$

$$a_2 b_2 \cos(30^\circ) = 2\pi, \quad \text{or} \quad b_2 = \frac{4\pi}{\sqrt{3}a_2}$$

$$\boldsymbol{b}_1 = \frac{2\pi}{\sqrt{3}a_1}(\sqrt{3},-1) \quad \text{and} \quad \boldsymbol{b}_2 = \frac{4\pi}{\sqrt{3}a_1}(0,-1)$$

The angle between $\boldsymbol{a}_1$ and $\boldsymbol{b}_1$ is 30º. The angle between $\boldsymbol{a}_2$ and $\boldsymbol{b}_2$ is 30º.

5.3 Graphite 2D lattice (honeycomb)

There are two atoms per cell. The lattice constant *a* is equal to 2.46 Å.

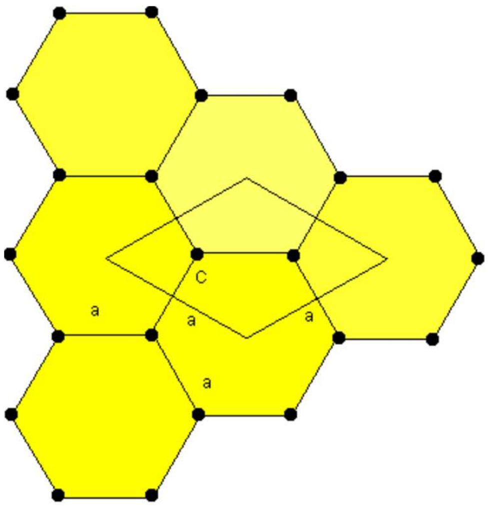


Fig. Two dimensional lattice for graphite layer (honeycomb). There are two carbon C atoms per unit cell.

The lattice constant of graphite is $a = 2.46$ Å. The graphite has a A-B stacking sequence along the c axis. We now consider the reciprocal lattice plane of the graphite lattice. The vectors $\boldsymbol{a}_1$ and $\boldsymbol{a}_2$ are the in-plane lattice vectors. The vectors $\boldsymbol{b}_1$ and $\boldsymbol{b}_2$ are the reciprocal lattice vectors. Note that $\boldsymbol{a}_1 \cdot \boldsymbol{b}_2 = 0$ and $\boldsymbol{a}_2 \cdot \boldsymbol{b}_1 = 0$. The angle between $\boldsymbol{a}_1$ and $\boldsymbol{b}_1$ is 30º.

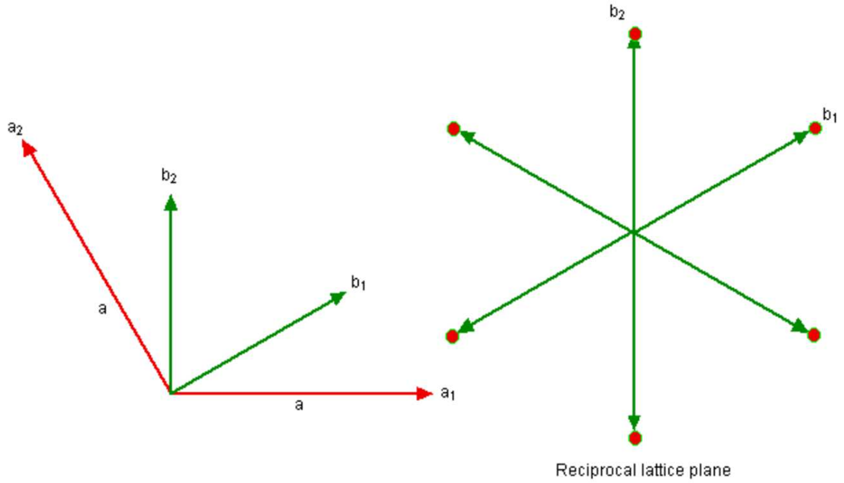


Fig. In-plane structure and the corresponding reciprocal lattice of the graphite lattice. $a_1 = 2.46$ Å. $b_1 = 4\pi/(\sqrt{3}a_1) = 2.95$ Å^{-1}.

$$\boldsymbol{a}_1 \cdot \boldsymbol{b}_1 = \boldsymbol{a}_2 \cdot \boldsymbol{b}_2 = 2\pi$$

$$a_1 b_1 \cos(30^\circ) = 2\pi, \quad \text{or} \quad b_1 = \frac{4\pi}{\sqrt{3}a_1} = 2.95 \text{ Å}^{-1}.$$

$$a_2 b_2 \cos(30^\circ) = 2\pi, \quad \text{or} \quad b_2 = \frac{4\pi}{\sqrt{3}a_2} = 2.95 \text{ Å}^{-1}.$$

6. 3D Reciprocal lattice vector

6.1 Definition

The reciprocal lattice vector $\boldsymbol{G}$ is expressed by

$$\boldsymbol{G} = k\boldsymbol{b}_1 + k\boldsymbol{b}_2 + l\boldsymbol{b}_3 .$$

where h, k, and l are integers and

$$\boldsymbol{b}_1 = 2\pi \frac{\boldsymbol{a}_2 \times \boldsymbol{a}_3}{[\boldsymbol{a}_1, \boldsymbol{a}_2, \boldsymbol{a}_3]}, \qquad \boldsymbol{b}_2 = 2\pi \frac{\boldsymbol{a}_3 \times \boldsymbol{a}_1}{[\boldsymbol{a}_1, \boldsymbol{a}_2, \boldsymbol{a}_3]}, \qquad \boldsymbol{b}_3 = 2\pi \frac{\boldsymbol{a}_1 \times \boldsymbol{a}_2}{[\boldsymbol{a}_1, \boldsymbol{a}_2, \boldsymbol{a}_3]}.$$

Note that

$$\boldsymbol{G} \cdot \boldsymbol{T} = (h\boldsymbol{b}_1 + k\boldsymbol{b}_2 + l\boldsymbol{b}_3) \cdot (u_1\boldsymbol{a}_1 + u_2\boldsymbol{a}_2 + u_3\boldsymbol{a}_3) = 2\pi(hu_1 + ku_2 + lu_3) .$$

We also note that

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

where δ_{ij} is the Kronecker delta function. We note that

$\boldsymbol{b}_1 \perp \boldsymbol{a}_2, \boldsymbol{a}_3$ ($\boldsymbol{b}_1$ is perpendicular to $\boldsymbol{a}_2$ and $\boldsymbol{a}_3$).

$\boldsymbol{b}_2 \perp \boldsymbol{a}_3, \boldsymbol{a}_1$ ($\boldsymbol{b}_2$ is perpendicular to $\boldsymbol{a}_3$ and $\boldsymbol{a}_1$).

$\boldsymbol{b}_3 \perp \boldsymbol{a}_1, \boldsymbol{a}_2$ ($\boldsymbol{b}_3$ is perpendicular to $\boldsymbol{a}_1$ and $\boldsymbol{a}_2$).

6. Reciprocal lattice vector: Simple cubic (sc) structure (primitive cell)

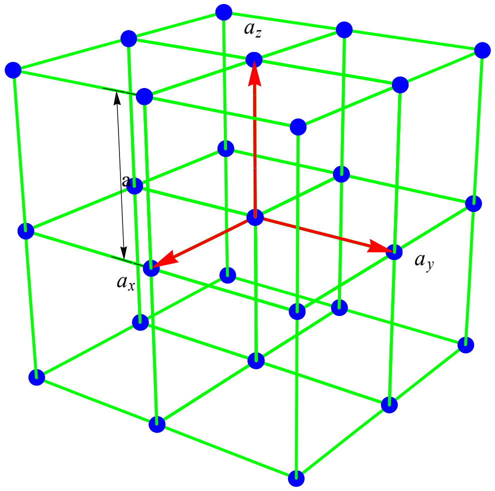


Fig. Crystal structure of sc system. $\boldsymbol{a}_x$, $\boldsymbol{a}_y$ and $\boldsymbol{a}_z$ are the primitive lattice vectors. The lattice constant is *a*.

The primitive translation vectors for sc are given by

$$\boldsymbol{a}_x = a(1,0,0), \qquad \boldsymbol{a}_y = a(0,1,0), \qquad \boldsymbol{a}_z = a(0,0,1),$$

with

$$\boldsymbol{a}_x \cdot (\boldsymbol{a}_y \times \boldsymbol{a}_z) = a^3 .$$

The corresponding reciprocal lattice vectors are

$$\boldsymbol{b}_x = \frac{2\pi(\boldsymbol{a}_y \times \boldsymbol{a}_z)}{\boldsymbol{a}_x \cdot (\boldsymbol{a}_y \times \boldsymbol{a}_z)} = \frac{2\pi}{a}(1,0,0),$$

$$\boldsymbol{b}_y = \frac{2\pi(\boldsymbol{a}_z \times \boldsymbol{a}_x)}{\boldsymbol{a}_x \cdot (\boldsymbol{a}_y \times \boldsymbol{a}_z)} = \frac{2\pi}{a}(0,1,0),$$

$$\boldsymbol{b}_z = \frac{2\pi(\boldsymbol{a}_x \times \boldsymbol{a}_y)}{\boldsymbol{a}_x \cdot (\boldsymbol{a}_y \times \boldsymbol{a}_z)} = \frac{2\pi}{a}(0,0,1).$$

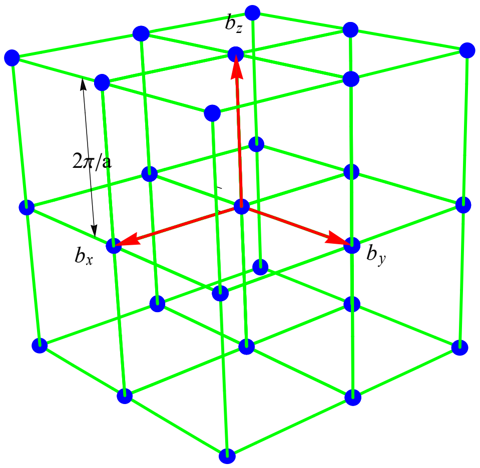
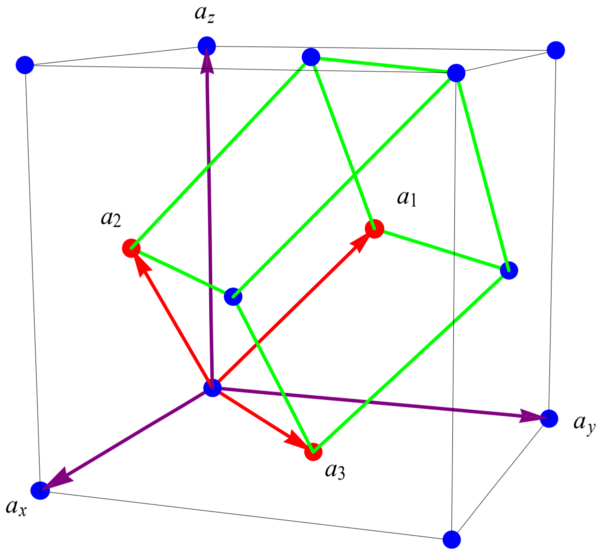


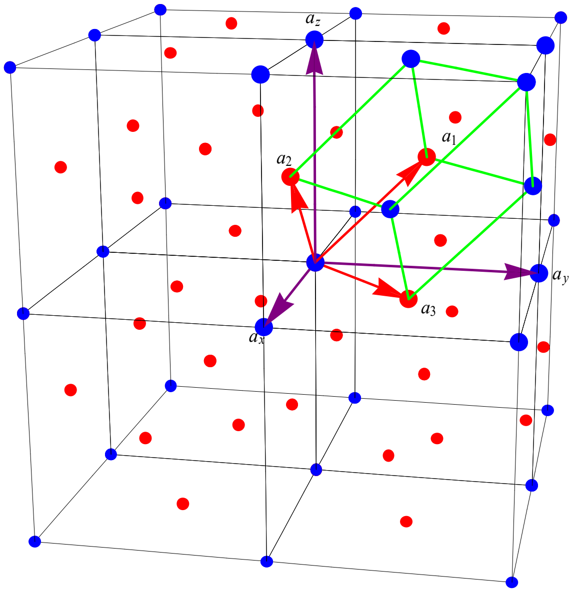
Fig.23 Reciprocal lattice points for the scc lattice. The vectors $\boldsymbol{b}_x$, $\boldsymbol{b}_y$, and $\boldsymbol{b}_z$ are the reciprocal lattice vectors. $b_x = b_y = b_z = \dfrac{2\pi}{a}$.

---

7. Reciprocal lattice vector: face-centered cubic (fcc) lattice

The primitive cell by definition has only one lattice point, but the conventional fcc cell contains four lattice points. Note that the lattice point is defined as follows. The atomic arrangement in the crystal looks exactly the same to an observer at $\boldsymbol{r}'$ (one lattice point) as to an observer at $\boldsymbol{r}$ (another lattice point).





fcc structure

Fig. Translation vectors of the primitive unit cell and conventional unit cell for the fcc.

The primitive translation vectors of the fcc lattice are expressed by

$$\boldsymbol{a}_1 = \frac{1}{2}a(0,1,1)\,, \qquad \boldsymbol{a}_2 = \frac{1}{2}a(1,0,1)\,, \qquad \boldsymbol{a}_3 = \frac{1}{2}a(1,1,0)$$

where there is one lattice point (or atom) per this primitive cell. We can generate all the points of the fcc lattice is described by

$$\boldsymbol{l} = l_1\boldsymbol{a}_1 + l_2\boldsymbol{a}_2 + l_3\boldsymbol{a}_3$$

with l_1, l_2, and l_3 integers. The volume of the primitive cell is

$$\boldsymbol{a}_1 \cdot (\boldsymbol{a}_2 \times \boldsymbol{a}_3) = \frac{a^3}{4}\,.$$

The corresponding reciprocal lattice vectors are given by

$$\boldsymbol{b}_1 = \frac{2\pi(\boldsymbol{a}_2 \times \boldsymbol{a}_3)}{\boldsymbol{a}_1 \cdot (\boldsymbol{a}_2 \times \boldsymbol{a}_3)} = \frac{2\pi}{a}(-1,1,1)$$

$$\boldsymbol{b}_2 = \frac{2\pi(\boldsymbol{a}_3 \times \boldsymbol{a}_1)}{\boldsymbol{a}_1 \cdot (\boldsymbol{a}_2 \times \boldsymbol{a}_3)} = \frac{2\pi}{a}(1,-1,1)$$

$$\boldsymbol{b}_3 = \frac{2\pi(\boldsymbol{a}_1 \times \boldsymbol{a}_2)}{\boldsymbol{a}_1 \cdot (\boldsymbol{a}_2 \times \boldsymbol{a}_3)} = \frac{2\pi}{a}(1,1,-1)$$

The reciprocal lattice vector is described by

$$\boldsymbol{G} = g_1\boldsymbol{b}_1 + g_2\boldsymbol{b}_2 + g_3\boldsymbol{b}_3 = \frac{2\pi}{a}(-g_1 + g_2 + g_3, g_1 - g_2 + g_3, g_1 + g_2 - g_3)$$

where g_1, g_2, and g_3 are integers. The translation vectors of the conventional unit cell (cubic) are expressed by

$$\boldsymbol{a}_x = a(1,0,0), \qquad \boldsymbol{a}_y = a(0,1,0), \qquad \boldsymbol{a}_z = a(0,0,1)$$

where there are two atoms per this conventional unit cell. The volume of the cubic cell is

$$\boldsymbol{a}_x \cdot (\boldsymbol{a}_y \times \boldsymbol{a}_z) = \frac{a^3}{4}.$$

The reciprocal lattice vectors are defined by

$$\boldsymbol{b}_x = \frac{2\pi(\boldsymbol{a}_y \times \boldsymbol{a}_z)}{\boldsymbol{a}_x \cdot (\boldsymbol{a}_y \times \boldsymbol{a}_z)} = \frac{2\pi}{a}(1,0,0)$$

$$\boldsymbol{b}_y = \frac{2\pi(\boldsymbol{a}_z \times \boldsymbol{a}_x)}{\boldsymbol{a}_x \cdot (\boldsymbol{a}_y \times \boldsymbol{a}_z)} = \frac{2\pi}{a}(0,1,0)$$

$$\boldsymbol{b}_z = \frac{2\pi(\boldsymbol{a}_x \times \boldsymbol{a}_y)}{\boldsymbol{a}_x \cdot (\boldsymbol{a}_y \times \boldsymbol{a}_z)} = \frac{2\pi}{a}(0,0,1)$$

In general, the reciprocal lattice vector is given by

$$\boldsymbol{G} = g_x\boldsymbol{b}_x + g_y\boldsymbol{b}_y + g_z\boldsymbol{b}_x = \frac{2\pi}{a}(g_x, g_y, g_z)$$

with

$$g_x = -g_1 + g_2 + g_3$$
$$g_y = g_1 - g_2 + g_3$$
$$g_z = g_1 + g_2 - g_3$$

There are relations between (g_x, g_y, g_z) and (g_1, g_2, g_3). Note that all indices of (g_x, g_y, g_z) are odd or even. There is a selection rule for the indices (g_x, g_y, g_z).

g_x	g_y	g_z	g_1	g_2	g_3
1	1	1	1	1	1
2	0	0	0	1	1
2	2	0	1	1	2
3	1	1	1	2	2
2	2	2	2	2	2
4	0	0	0	2	2
3	3	1	2	2	3
4	2	0	1	2	3
4	2	2	2	3	3
5	1	1	1	3	3

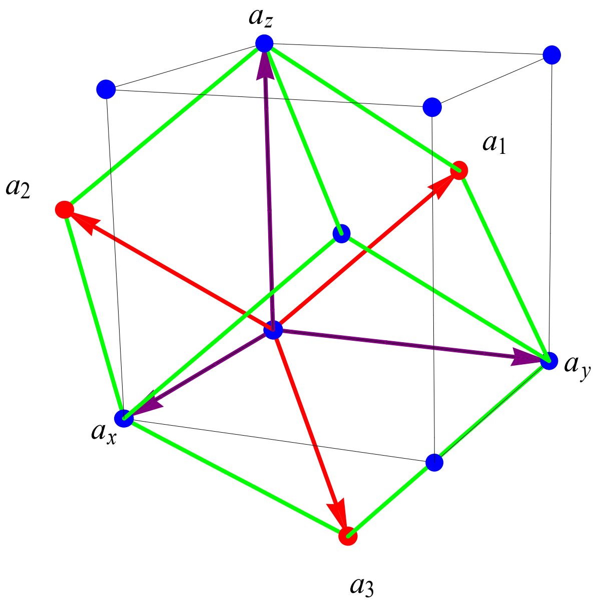
Selection rule for the indices (g_x, g_y, g_z) for fcc.

((Note))
For fcc structure, it is required that

$$g_x^2 + g_y^2 + g_z^2 = 3, 4, 8, 11, 12, 16, 19, 20, 24, 27, 32, 35, 40, 36, 43, 44, 48$$

9. Reciprocal lattice vector: body-centered cubic (bcc) structure

The primitive cell by definition contains only one lattice point, but the conventional bcc cell contains two lattice points.



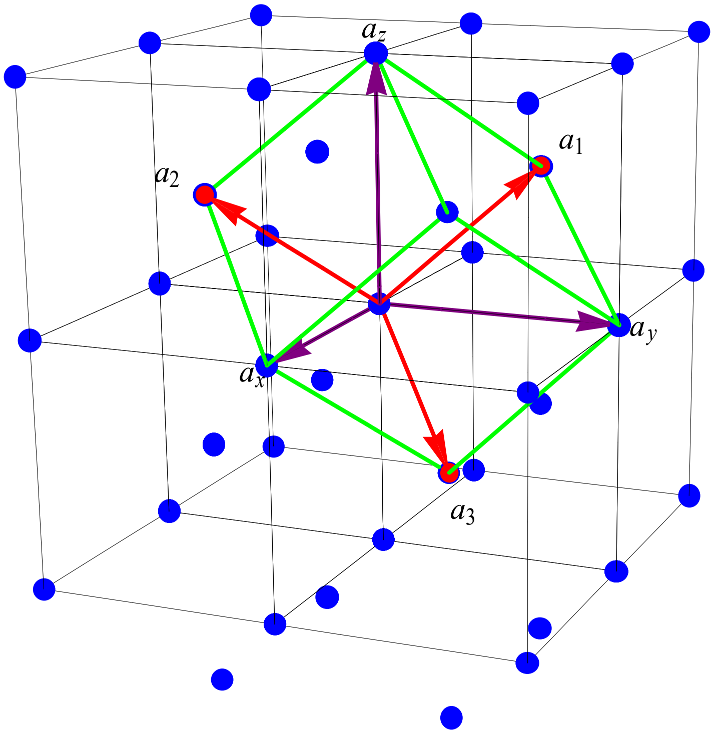


Fig.

The primitive translation vectors of the bcc lattice are expressed by

$$\boldsymbol{a}_1 = \frac{1}{2}a(-1,1,1)\,, \qquad \boldsymbol{a}_2 = \frac{1}{2}a(1,-1,1)\,, \qquad \boldsymbol{a}_3 = \frac{1}{2}a(1,1,-1)$$

where there is one atom per this primitive cell. We can generate all the points of the bcc lattice is described by

$$\boldsymbol{l} = l_1\boldsymbol{a}_1 + l_2\boldsymbol{a}_2 + l_3\boldsymbol{a}_3$$

with l_1, l_2, and l_3 integers. The volume of the primitive cell is

$$\boldsymbol{a}_1 \cdot (\boldsymbol{a}_2 \times \boldsymbol{a}_3) = \frac{a^3}{2}$$

The corresponding reciprocal lattice vectors are given by

$$\boldsymbol{b}_1 = \frac{2\pi(\boldsymbol{a}_2 \times \boldsymbol{a}_3)}{\boldsymbol{a}_1 \cdot (\boldsymbol{a}_2 \times \boldsymbol{a}_3)} = \frac{2\pi}{a}(0,1,1)$$

$$\boldsymbol{b}_2 = \frac{2\pi(\boldsymbol{a}_3 \times \boldsymbol{a}_1)}{\boldsymbol{a}_1 \cdot (\boldsymbol{a}_2 \times \boldsymbol{a}_3)} = \frac{2\pi}{a}(1,0,1)$$

$$\boldsymbol{b}_3 = \frac{2\pi(\boldsymbol{a}_1 \times \boldsymbol{a}_2)}{\boldsymbol{a}_1 \cdot (\boldsymbol{a}_2 \times \boldsymbol{a}_3)} = \frac{2\pi}{a}(1,1,0)$$

The reciprocal lattice vector is described by

$$\boldsymbol{G} = g_1\boldsymbol{b}_1 + g_2\boldsymbol{b}_2 + g_3\boldsymbol{b}_3 = \frac{2\pi}{a}(g_2 + g_3, g_1 + g_3, g_1 + g_2)$$

where g_1, g_2, and g_3 are integers.

The translation vectors of the conventional unit cell are expressed by

$$\boldsymbol{a}_x = a(1,0,0)\,, \qquad \boldsymbol{a}_y = a(0,1,0)\,, \qquad \boldsymbol{a}_z = a(0,0,1)$$

where there are two atoms per this conventional unit cell. The reciprocal lattice vectors are defined by

$$\boldsymbol{b}_x = \frac{2\pi(\boldsymbol{a}_y \times \boldsymbol{a}_z)}{\boldsymbol{a}_x \cdot (\boldsymbol{a}_y \times \boldsymbol{a}_z)} = \frac{2\pi}{a}(1,0,0)$$

$$\boldsymbol{b}_y = \frac{2\pi(\boldsymbol{a}_z \times \boldsymbol{a}_x)}{\boldsymbol{a}_x \cdot (\boldsymbol{a}_y \times \boldsymbol{a}_z)} = \frac{2\pi}{a}(0,1,0)$$

$$\boldsymbol{b}_z = \frac{2\pi(\boldsymbol{a}_x \times \boldsymbol{a}_y)}{\boldsymbol{a}_x \cdot (\boldsymbol{a}_y \times \boldsymbol{a}_z)} = \frac{2\pi}{a}(0,1,0)$$

The reciprocal lattice vector is given by

$$\boldsymbol{G} = g_x \boldsymbol{b}_x + g_y \boldsymbol{b}_y + g_z \boldsymbol{b}_x = \frac{2\pi}{a}(g_x, g_y, g_z)$$

with

$$\begin{aligned} g_x &= g_2 + g_3 \\ g_y &= g_1 + g_3 \\ g_z &= g_1 + g_2 \end{aligned}$$

There are relations between (g_x, g_y, g_z) and (g_1, g_2, g_3). Note that

$$g_x + g_y + g_z = 2(g_1 + g_2 + g_3)$$

which is even.

g_x	g_y	g_z	g_1	g_2	g_3
1	1	0	0	0	1
2	0	0	-1	1	1
2	1	1	0	1	1
2	2	0	0	0	2
3	1	0	-1	1	2
2	2	2	1	1	1
3	2	1	0	1	2
4	0	0	-2	2	2

Selection rule for the indices (g_x, g_y, g_z) for the cubic bcc

For bcc structure, it is required that

$$g_x^2 + g_y^2 + g_z^2 = 2, 4, 6, 8, 10, 12, 14, 16, 18, 20, 22, 24, '$$

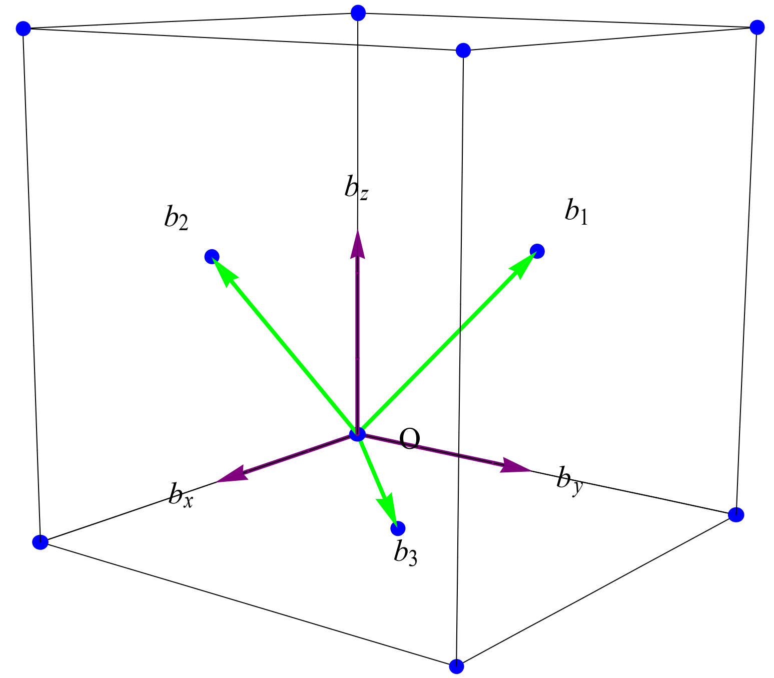


Fig.

The reciprocal lattice vectors, $\boldsymbol{b}_1$, $\boldsymbol{b}_2$, and $\boldsymbol{b}_3$ for the primitive cell and $\boldsymbol{b}_x$, $\boldsymbol{b}_y$, and $\boldsymbol{b}_z$ for the cubic cell (conventional cell) for the bcc lattice. The reciprocal lattice points (denoted by solid blue circles) are located on a fcc lattice with

11. Origin of the Reciprocal lattice vector

For simplicity we discuss the case of one dimension (1D). We consider the Fourier transform of the number density of electrons in the periodic lattice. In the free space, the electron propagating to the positive x direction, has the form of plane wave as a wave function,

$$\psi_k = e^{ikx}$$

In free space, the number density $n(x)$ of electrons can be expressed by the superposition of the plane waves with any wave number k. Here we assume the duality of wave and particle in quantum mechanics. In this case, using the Fourier transform, $n(x)$ can be expressed by

$$n(x) = \sum_k n_k e^{ikx}$$

Suppose that the electrons are in the quantum box with the size L. The wave number k is not continuous any more. When we use the periodic boundary condition,

$$e^{ik(x+L)} = e^{ikx}$$

or

$$e^{ikL} = 1$$

or

$$k = \frac{2\pi m}{L} = \frac{2\pi m}{Na} = \frac{2\pi}{a}\frac{m}{N} \qquad (n\text{: integer})$$

where $L = Na$, and *m*, and *N* are integer numbers. Thus the number density of electrons is rewritten by

$$n(x) = \sum_m n_m e^{i\frac{2\pi}{a}\frac{m}{N}x}$$

Now we assume the periodic condition that

$$n(x+a) = n(x)$$

Then we get

$$\begin{aligned} n(x+a) &= \sum_m n_m e^{i\frac{2\pi}{a}\frac{m}{N}(x+a)} \\ &= \sum_m e^{i\frac{2\pi}{a}\frac{m}{N}a} n_m e^{i\frac{2\pi}{a}\frac{m}{N}x} \\ &= \sum_m e^{i2\pi\frac{m}{N}} n_m e^{i\frac{2\pi}{a}\frac{m}{N}x} \\ &= n(x) \end{aligned}$$

In order to have the above condition, we need the condition for m,

$$m = sN \, (s = 0, \ \pm 1, \pm 2, \pm 3, \dots).$$

The final expression for $n(x)$ is

$$n(x) = \sum_s n_s e^{i\frac{2\pi}{a}sx} = \sum_G n_G e^{iGx}$$

where *G* is the reciprocal lattice

$$G = \frac{2\pi}{a} \qquad \text{(the minimum value)}$$

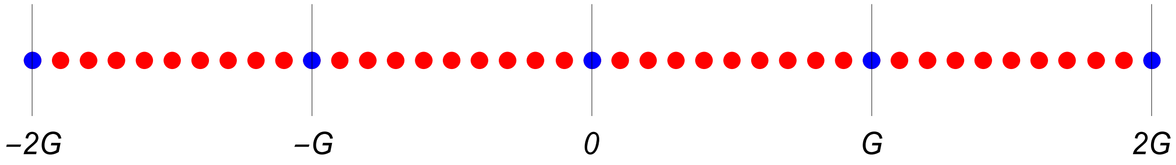


Fig. The distribution of wave number k in the 1D system. The discreteness of k (the separation $2\pi / L$) comes from the size of the system L. The blue points denote the reciprocal lattice points G which is equal to integer times $2\pi/a$, where a is the lattice constant (the space periodicity)

This means that only the plane wave with the wave number of the reciprocal lattice contributes to the number density of electrons in a periodic lattice. This discussion can be extended to both the 2D and 3D systems. In general, we have

$$n(\boldsymbol{r}) = \sum_{\boldsymbol{G}} n_{\boldsymbol{G}} e^{i\boldsymbol{G}\cdot\boldsymbol{r}}$$

with the reciprocal lattice vector

$$\boldsymbol{G} = h\boldsymbol{b}_1 + k\boldsymbol{b}_2 + l\boldsymbol{b}_3$$

where $\boldsymbol{a}_i \cdot \boldsymbol{b}_j = 2\pi\delta_{i,,j}$.For any translation vector

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

we have $n(\boldsymbol{r})$ satisfies the periodic condition,

$$\begin{aligned} n(\boldsymbol{r}+\boldsymbol{T}) &= \sum_{\boldsymbol{G}} n_{\boldsymbol{G}} e^{i\boldsymbol{G}\cdot(\boldsymbol{r}+\boldsymbol{T})} \\ &= \sum_{\boldsymbol{G}} e^{i\boldsymbol{G}\cdot\boldsymbol{T}} n_{\boldsymbol{G}} e^{i\boldsymbol{G}\cdot\boldsymbol{r}} \\ &= n(\boldsymbol{r}) \end{aligned}$$

Note that $e^{i\boldsymbol{G}\cdot\boldsymbol{T}} = 1$, since

$$\begin{aligned} \boldsymbol{G}\cdot\boldsymbol{T} &= (h\boldsymbol{b}_1 + k\boldsymbol{b}_2 + l\boldsymbol{b}_3)\cdot(u_1\boldsymbol{a}_1 + u_2\boldsymbol{a}_2 + u_3\boldsymbol{a}_3) \\ &= 2\pi(hu_1 + ku_2 + lu_3) \end{aligned}$$

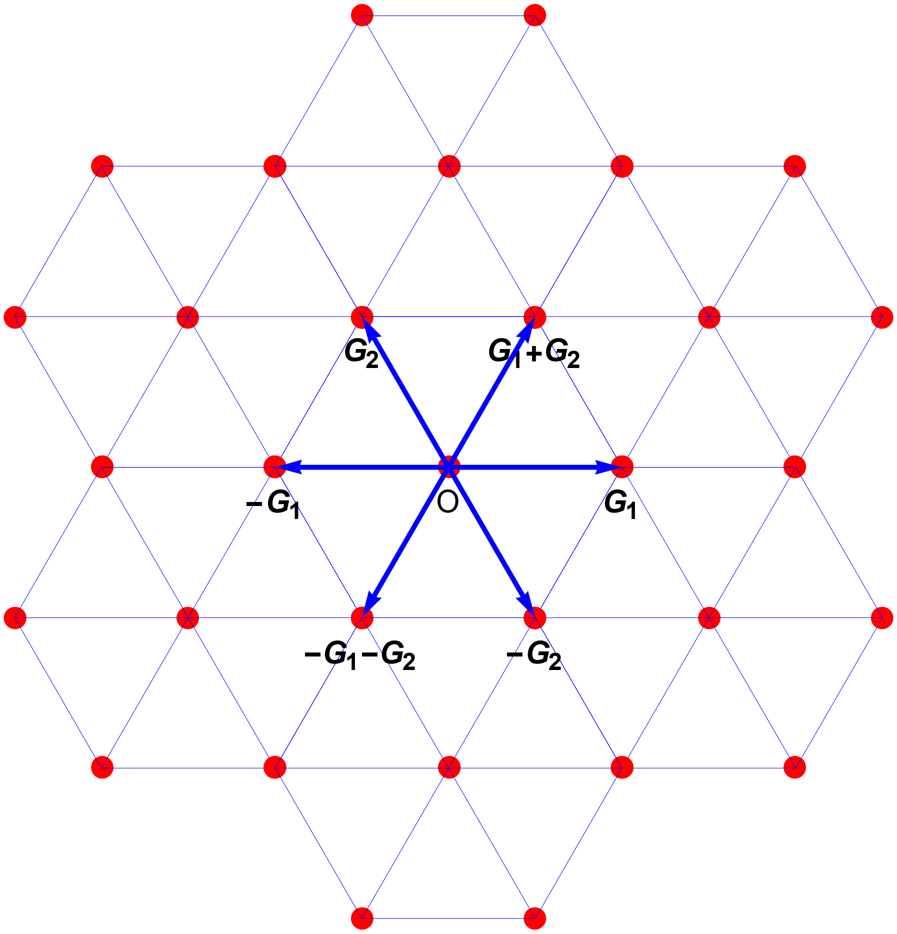


Fig. Reciprocal lattice plane for the 2D hexagonal lattice.

12. Electron density: Fourier analysis

A crystal is invariant under any translation of the form

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

where u_1, u_2, u_3 are integers and $\boldsymbol{a}_1$, $\boldsymbol{a}_2$, $\boldsymbol{a}_3$ are the periods along the crystal axes. Any local physical property of the crystal is invariant under $\boldsymbol{T}$: charge concentration, electron number, magnetic moment density. Electron number density $n(\boldsymbol{r})$ is a periodic function of $\boldsymbol{r}$, with periods $\boldsymbol{a}_1$, $\boldsymbol{a}_2$, $\boldsymbol{a}_3$ in the directions of the three axes.

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

We consider the Fourier series

$$n(\boldsymbol{r}) = \sum_{\boldsymbol{G}} n_G \exp(i\boldsymbol{G}\cdot\boldsymbol{r})$$

$$n(\boldsymbol{r}+\boldsymbol{T}) = \sum_{\boldsymbol{G}} n_G \exp[i\boldsymbol{G}\cdot(\boldsymbol{r}+\boldsymbol{T})] = \exp[i\boldsymbol{G}\cdot\boldsymbol{T})]\sum_{\boldsymbol{G}} n_G \exp(i\boldsymbol{G}\cdot\boldsymbol{r}) = n(\boldsymbol{r})$$

or

$\boldsymbol{G}\cdot\boldsymbol{T} = 2\pi$ x integer

The extension of the Fourier analysis to periodic function $n(\boldsymbol{r})$ in the 3D,

$$n(\boldsymbol{r}) = \sum_{\boldsymbol{G}} n_G \exp(i\boldsymbol{G}\cdot\boldsymbol{r})$$

where $\boldsymbol{G}$ is the reciprocal lattice vectors, and n_{G} determine the x-ray scattering amplitude. $\boldsymbol{G}$ is described by

$$\boldsymbol{G} = h\boldsymbol{b}_1 + k\boldsymbol{b}_2 + l\boldsymbol{b}_3$$

where h, k, and l are integers. $\boldsymbol{b}_1$, $\boldsymbol{b}_2$, and $\boldsymbol{b}_3$ need to satisfy the condition

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

where δ_{ij} is the Kronecker delta symbol: δ_{ij} = 1 for $i = j$ and δ_{ij} = 0 for $i = j$. Then we have

$$\boldsymbol{G}\cdot\boldsymbol{T} = (h\boldsymbol{b}_1 + k\boldsymbol{b}_2 + l\boldsymbol{b}_3)\cdot(u_1\boldsymbol{a}_1 + u_2\boldsymbol{a}_2 + u_3\boldsymbol{a}_3) = 2\pi(hu_1 + ku_2 + lu_3)$$

13. Fourier component n_{G} and the structure factor S_{G}.

We now calculate the Fourier component n_{G}.

$$\int_V n(\boldsymbol{r})e^{-i\boldsymbol{G}\cdot\boldsymbol{r}}d\boldsymbol{r} = \int_V \sum_{\boldsymbol{G}'} n_{\boldsymbol{G}'}e^{i\boldsymbol{G}'\cdot\boldsymbol{r}}e^{-i\boldsymbol{G}\cdot\boldsymbol{r}}d\boldsymbol{r} = \sum_{\boldsymbol{G}'} n_{\boldsymbol{G}'}\int e^{i(\boldsymbol{G}'-\boldsymbol{G})\cdot\boldsymbol{r}}d\boldsymbol{r} = n_{\boldsymbol{G}}V$$

where $\int e^{i(\boldsymbol{G}'-\boldsymbol{G})\cdot\boldsymbol{r}}d\boldsymbol{r} = V\delta_{\boldsymbol{G}',\boldsymbol{G}}$, and V is the total volume of the system. So we get

$$n_{\boldsymbol{G}} = \frac{1}{V}\int_V n(\boldsymbol{r})e^{-i\boldsymbol{G}\cdot\boldsymbol{r}}d\boldsymbol{r}$$

where N is the total number of atoms and $V = NV_{cell}$.

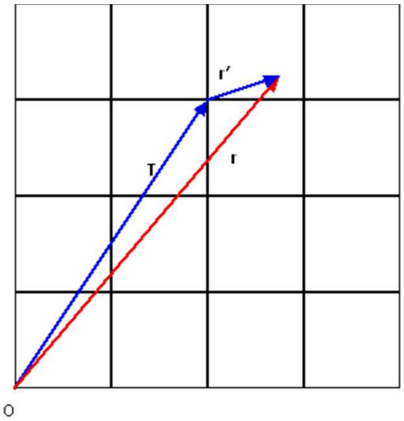


Fig. System consisting of periodic cells. ***T*** is the translation vector. $\boldsymbol{r} = \boldsymbol{T} + \boldsymbol{r}'$.

Since

$$\boldsymbol{r} = \boldsymbol{T} + \boldsymbol{r}',$$

we get

$$n(\boldsymbol{r}) = n(\boldsymbol{T} + \boldsymbol{r}') = n(\boldsymbol{r}').$$

We also note that

$$e^{-i\boldsymbol{G}\cdot\boldsymbol{r}} = e^{-i\boldsymbol{G}\cdot(\boldsymbol{r}'+\boldsymbol{T})} = e^{-i\boldsymbol{G}\cdot\boldsymbol{r}'}.$$

Then we have

$$n_{\boldsymbol{G}} = \frac{1}{NV_{cell}}[N\int_{V_{cell}} n(\boldsymbol{r})e^{-i\boldsymbol{G}\cdot\boldsymbol{r}}d\boldsymbol{r}] = \frac{1}{V_{cell}}\int_{V_{cell}} n(\boldsymbol{r})e^{-i\boldsymbol{G}\cdot\boldsymbol{r}}d\boldsymbol{r}$$

Here we define the structure factor as

$$S_{\boldsymbol{G}} = \int_{V_{cell}} n(\boldsymbol{r})e^{-i\boldsymbol{G}\cdot\boldsymbol{r}}d\boldsymbol{r}$$

or

$$n_{\mathbf{G}} = \frac{1}{V_{cell}} S_{\mathbf{G}}$$

14. One dimensional case

For simplicity, we consider a function $n(x)$ with a period a in the x direction (one dimensional case).

$$n(x) = n(x+a)$$

Suppose that $n(x)$ may be expressed by

$$n(x) = \sum_g n_g \exp(igx)$$

$$n(x+a) = \sum_g n_g \exp[ig(x+a)] = \exp(iga) \sum_g n_g \exp(igx) = \exp(iga) n(x) = n(x)$$

Then we have

$$\exp(iga) = 1$$

or

$$g = \frac{2\pi}{a} l$$

Thus we have

$$n(x) = \sum_g n_g \exp(igx)$$

with

$$n_g = \frac{1}{a} \int_0^a dx n(x) e^{-igx}$$

((**Example-1**)) What is the value of n_g? We consider the simplest case.

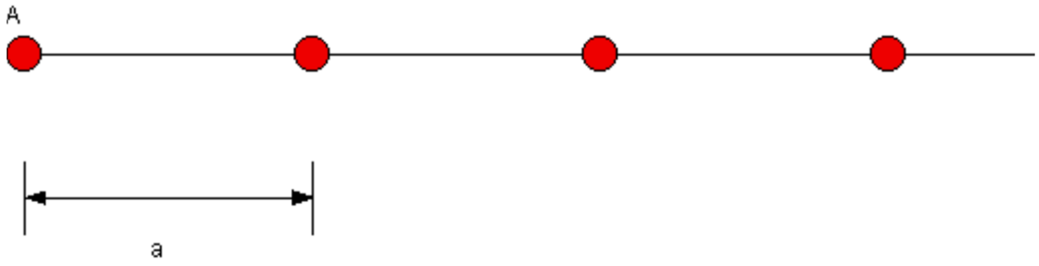


Fig. A simple one dimensional array with a lattice constant *a*.

$$n_g = \frac{1}{a}\int_0^a \delta(x)edx = \frac{1}{a}$$

with $g = \frac{2\pi}{a}l$

where $\delta(x)$ is the Dirac delta function.

((**Example 2**))

There are two atoms in each unit cell with the lattice constant *a*.

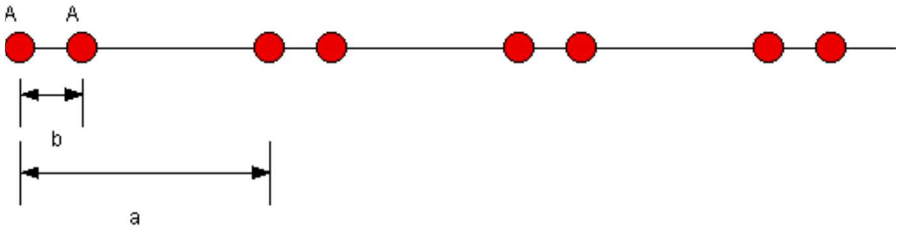


Fig. One dimensional array with to atoms per unit cell with a lattice constant *a*.

$$n_g = \frac{1}{a}\int_0^a [\delta(x) + \delta(x-b)]e^{-igx}dx = \frac{1}{a}(1 + e^{-igb})$$

$$\left|n_g\right|^2 = n_g n_g^{\ *} = \frac{(1+e^{-igb})(1+e^{igb})}{a^2} = \frac{4}{a^2}\cos^2(\frac{gb}{2})$$

with $g = \frac{2\pi}{a} l$

((**Mathematica**)): $\left| n_g \right|^2$ vs l where $a = 1$ and $b = 0.3$.

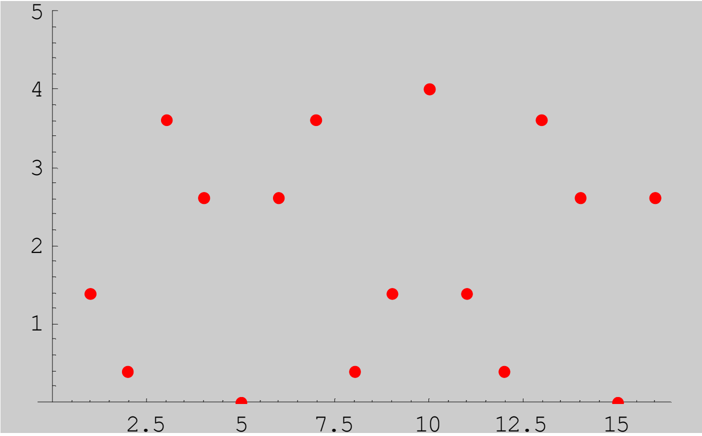


Fig. Intensity $\left| n_g \right|^2$ vs Bragg index l for the 1D system shown in Fig.22.

15. Structure factor

S_G is called the structural factor and defined as an integral over a single cell.

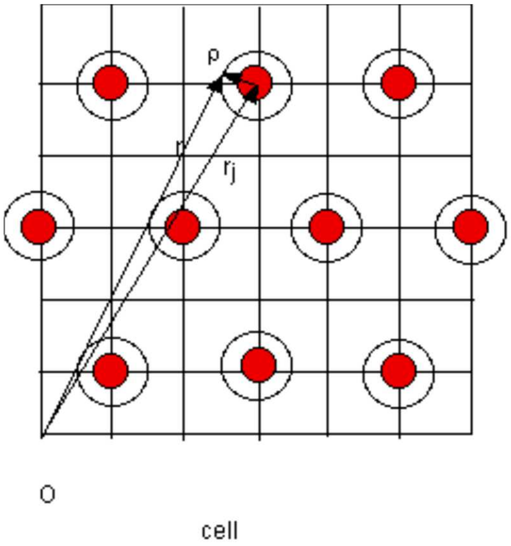


Fig. Unit cell having more than two atoms. $\boldsymbol{r} = \boldsymbol{r}_j + \boldsymbol{\rho}$.

Let $n_j(\boldsymbol{r} - \boldsymbol{r}_j)$ be defined by the contribution of atom j to the electron concentration.

$$n(\boldsymbol{r}) = \sum_{j=1}^{s} n_j(\boldsymbol{r} - r_j),$$

over the *s* atoms of the basis.

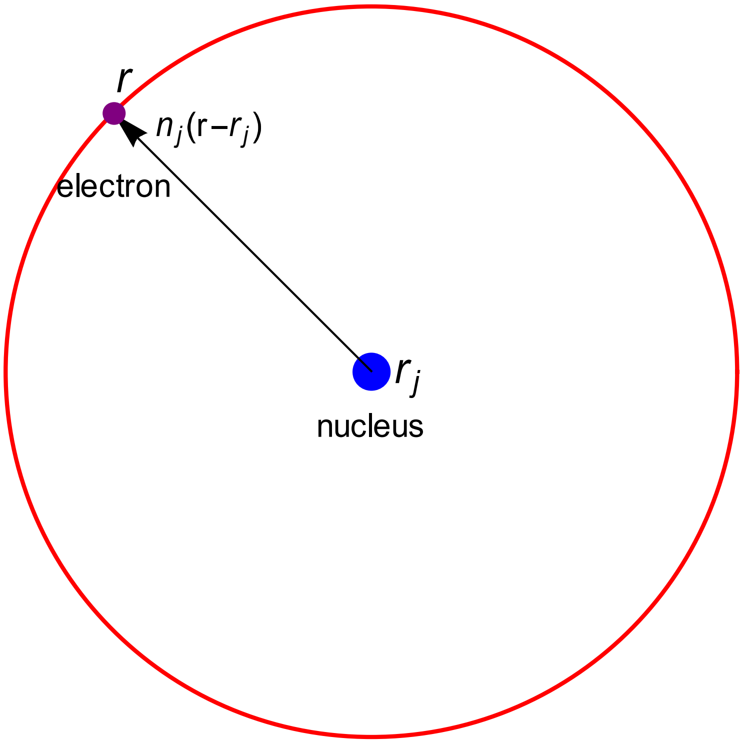


Fig. Electron distribution around the nucleus. $\boldsymbol{r} - \boldsymbol{r}_j = \boldsymbol{\rho}$

Then we have

$$S_{\boldsymbol{G}} = \int_{V_{cell}} n(\boldsymbol{r}) e^{-i\boldsymbol{G}\cdot\boldsymbol{r}} d\boldsymbol{r} = \sum_{j=1}^{s} \int_{V_{cell}} n_j(\boldsymbol{r} - \boldsymbol{r}_j) e^{-i\boldsymbol{G}\cdot\boldsymbol{r}} d\boldsymbol{r},$$

or

$$S_{\boldsymbol{G}} = \sum_j e^{-i\boldsymbol{G}\cdot\boldsymbol{r}_j} \int_{V_{cell}} n_j(\boldsymbol{\rho}) e^{-i\boldsymbol{G}\cdot\boldsymbol{\rho}} d\boldsymbol{\rho}.$$

where $\boldsymbol{r} = \boldsymbol{r}_j + \boldsymbol{\rho}$. We now define the *atomic form factor* as

$$f_j = \int_{V_{cell}} n_j(\boldsymbol{\rho}) e^{-i\boldsymbol{G}\cdot\boldsymbol{\rho}} d\boldsymbol{\rho} .$$

The atomic form factor is a measure of the scattering power of the *j*-th atom in the unit cell. The value of *f* involves the number and distribution of atomic electrons. Then S_G is given by the form

$$S_{\boldsymbol{G}} = \sum_j f_j e^{-i\boldsymbol{G}\cdot\boldsymbol{r}_j} .$$

The structure factor S_G need not to be real because the scattering intensity will involve

$$S_{\mathbf{G}} * S_{\mathbf{G}} = |S_{\mathbf{G}}|^2$$

where $S_{\boldsymbol{G}}^*$ is the complex conjugate of $S_{\mathbf{G}}$.

16. General expression for structure factor

The electron density is expressed by

$$n(\boldsymbol{r}) = \sum_{m,n,p} \sum_j f_j \delta(\boldsymbol{r} - \boldsymbol{r}_j - \boldsymbol{R}_{mnp})$$

where f_j is the atomic form factor. The Fourier transform of $n(\boldsymbol{r})$ is defined by

$$\begin{aligned} \int dV e^{-i\Delta\boldsymbol{k}\cdot\boldsymbol{r}} n(\boldsymbol{r}) &= \int dV e^{-i\Delta\boldsymbol{k}\cdot\boldsymbol{r}} \sum_{m,n,p} \sum_j f_j \delta(\boldsymbol{r} - \boldsymbol{r}_j - \boldsymbol{R}_{mnp}) \\ &= \sum_{m,n,p} e^{-i\Delta\boldsymbol{k}\cdot\boldsymbol{R}_{mnp}} \sum_j f_j e^{-i\Delta\boldsymbol{k}\cdot\boldsymbol{r}_j} \\ &= \sum_{\boldsymbol{G}} \delta(\Delta\boldsymbol{k} - \boldsymbol{G}) \sum_j f_j e^{-i\Delta\boldsymbol{k}\cdot\boldsymbol{r}_j} \\ &= \sum_{\boldsymbol{G}} \delta(\Delta\boldsymbol{k} - \boldsymbol{G}) \sum_j f_j e^{-i\boldsymbol{G}\cdot\boldsymbol{r}_j} \end{aligned}$$

where

$$\boldsymbol{R}_{mnp} = m\boldsymbol{a}_1 + n\boldsymbol{a}_2 + p\boldsymbol{a}_3$$

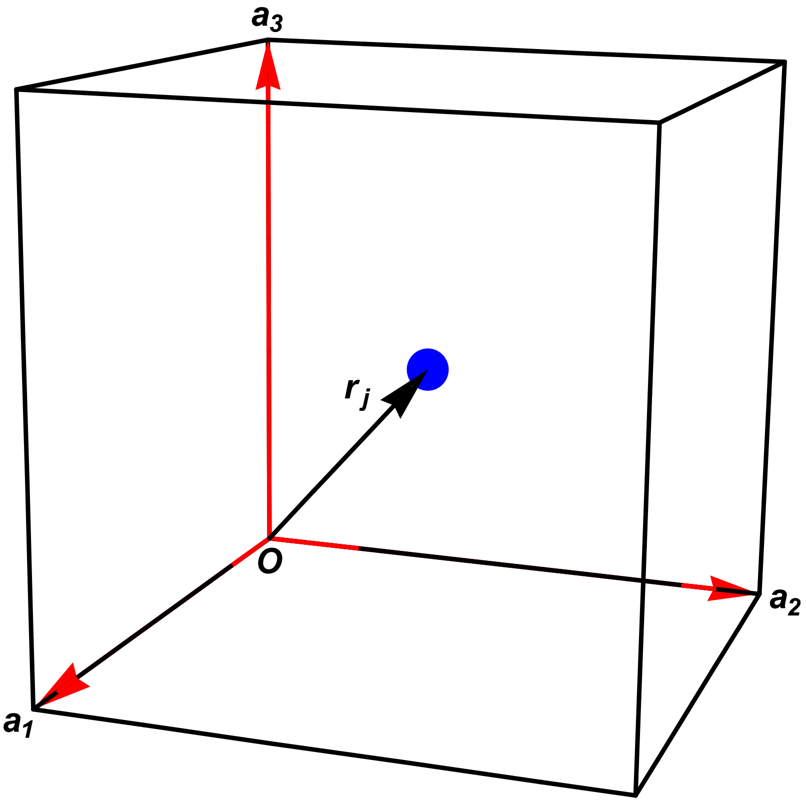


Fig. Position of the *j*-th atom within the unit cell is specified by r_j.

We note that the structure factor is defined by

$$S_G = \sum_j f_j e^{-i\boldsymbol{G}\cdot\boldsymbol{r}_j} \qquad \text{(structure factor)}$$

We also use the Poisson sum rule;

$$\sum_{m,n,p} e^{-i\Delta\boldsymbol{k}\cdot\boldsymbol{R}_{mnp}} = \sum_G \delta(\Delta\boldsymbol{k} - \boldsymbol{G})$$

17. Atomic form factor

When $\boldsymbol{G} = 0$, f_j is equal to the total number of electrons around the nucleus (Z)

$$f_j = \int_{V_{cell}} n_j(\boldsymbol{\rho})d\boldsymbol{\rho} = Z\,.$$

The value of *f* for atoms may be found in the international tables for x-ray crystallography. Suppose that the electron distribution is spherically symmetric about the origin:

$$n_j(\boldsymbol{\rho}) = n_j(\rho),$$

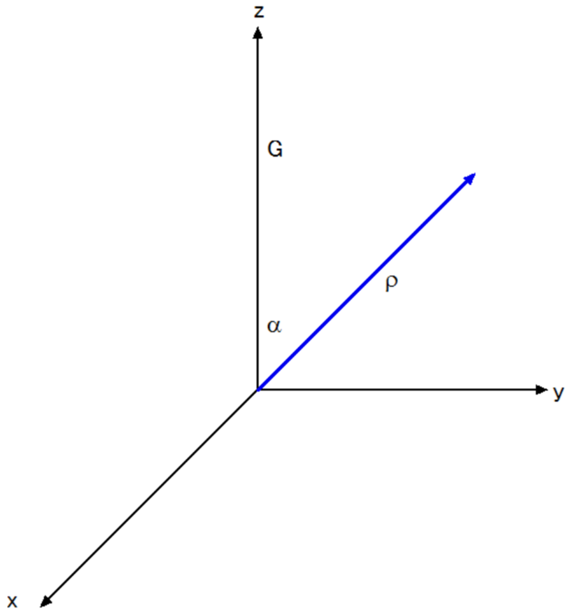


Fig. Relation between ***G*** and ρ in the Cartesian coordinates.

Let ρ make an angle α with ***G***. Then we get

$$\begin{aligned} f_j &= \int_0^\infty 2\pi\rho^2 n_j(\rho)d\rho\int_0^\pi \sin\alpha d\alpha e^{-iG\rho\cos\alpha} \\ &= \int_0^\infty 2\pi\rho^2 n_j(\rho)d\rho[\frac{1}{iG\rho}e^{-iG\rho\cos\alpha}]_0^\pi \\ &= \int_0^\infty \frac{2\pi\rho^2 n_j(\rho)}{iG\rho}d\rho(e^{iG\rho} - e^{-iG\rho}) \\ &= 4\pi\int_0^\infty d\rho\rho^2 n_j(\rho)\frac{\sin(G\rho)}{G\rho} \end{aligned}$$

$$f_j = 4\pi\int d\rho\rho^2 n_j(\rho)\frac{\sin(G\rho)}{G\rho}.$$

Then the atomic form factor is dependent on *G*. When *G* = 0, $\frac{\sin(G\rho)}{G\rho} = 1$;

$$f_j = 4\pi \int d\rho \rho^2 n_j(\rho) = Z ,$$

where Z is the number of atomic electrons. The atom has a size comparable to the wavelength of the x-rays., and scattered rays leaving different parts of the atomic charge cloud are not exactly in phase. The difference in phase is zero at zero diffraction angle, but increases markedly as the angle increases. The atomic factor thus decreases with the angle of diffraction.

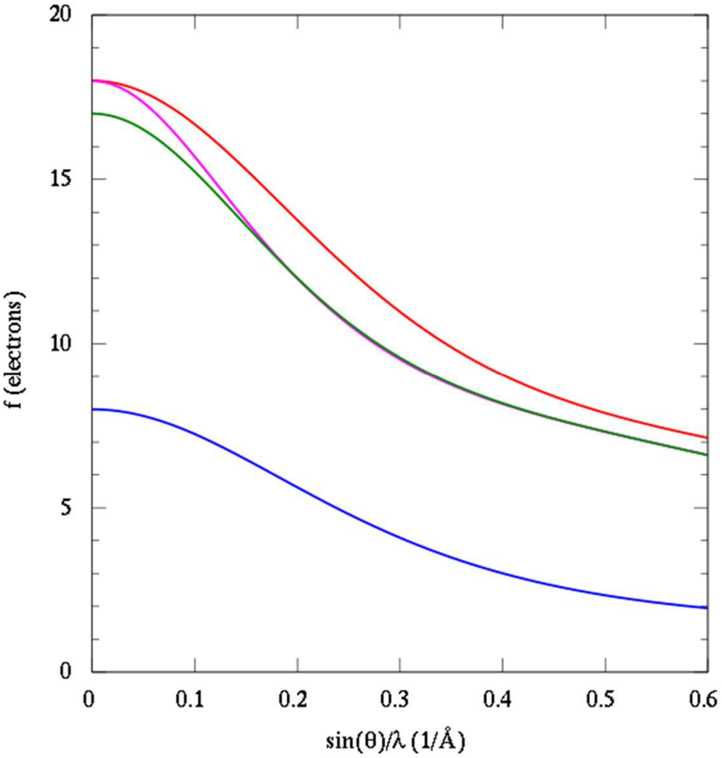


Fig. x-ray atomic form factors of oxygen (blue), chlorine (green), Cl^- (magenta), and K^+ (red); smaller charge distributions have a wider form factor. $\frac{\sin\theta}{\lambda} = \frac{Q}{4\pi} = \frac{G}{4\pi}$. In this Fig, f is plotted as a function of $G/4\pi$.

http://en.wikipedia.org/wiki/Atomic_form_factor

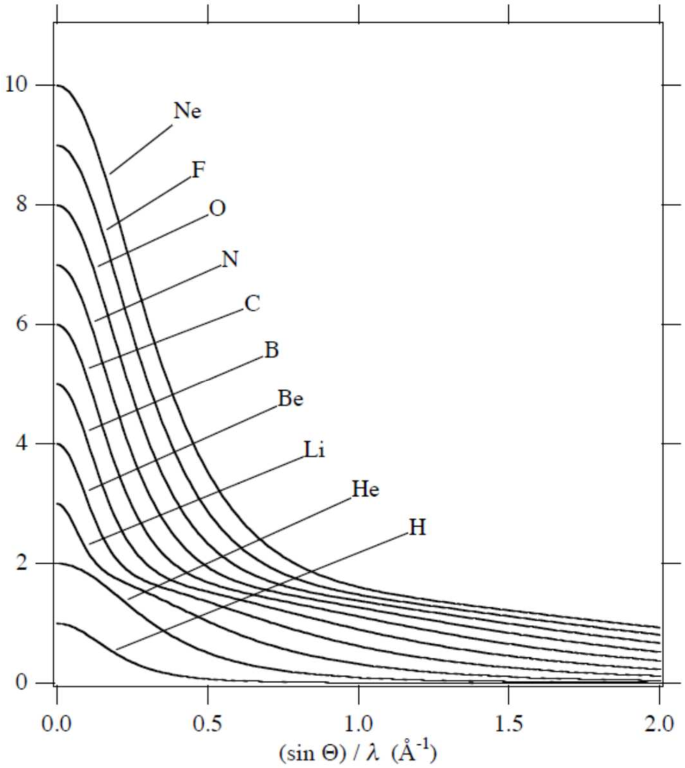


Fig. x-ray atomic form factors for H (Z = 1) to Ne (Z = 10). The atomic form factor tends to show tail to higher Q as Z increases. This means that the orbital radius of the inner shells become smaller for the larger charges of Ze of the nucleus.
http://www.crl.nitech.ac.jp/~ida/education/structureanalysis/3/3.pdf

((**Example**))
We now calculate the form factor of atomic hydrogen in the ground state. The number density is given by

$$n(\rho) = \frac{1}{\pi a_0^3} e^{-2r/a_0}.$$

where a_0 is the Bohr radius (a_0 = 0.53 Å)

$$f_G = \frac{16}{(4 + G^2 a_0{}^2)^2}.$$

((**Mathematica**))

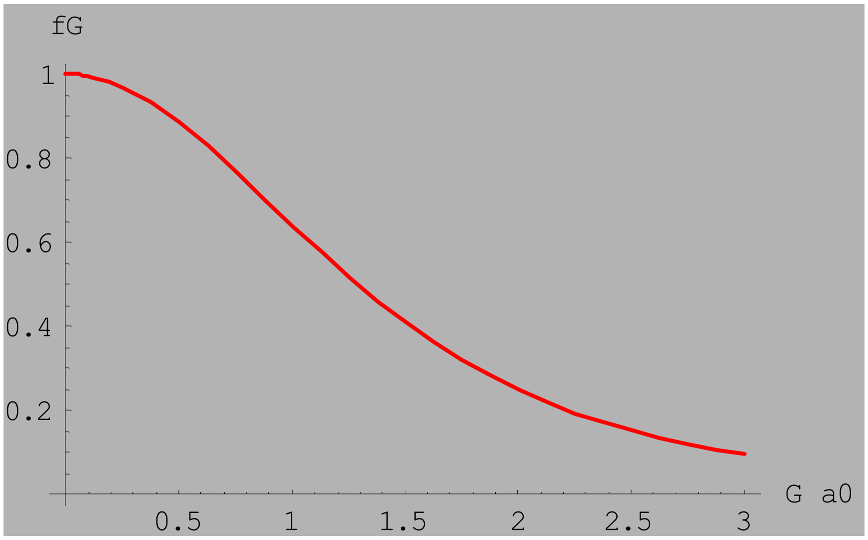


Fig. The atomic form factor of hydrogen in the ground state

18. The structure factor for 1D, 2D and 3D systems

18.1 One dimensional case

The structure factor for the 1D case is given by

$$S_{\boldsymbol{G}} = \int n(\boldsymbol{r}_{1D}) e^{-i\boldsymbol{G}\cdot\boldsymbol{r}_{1D}} d\boldsymbol{r}_{1D} = \int n(z) e^{-iG_z z} dz$$

where

$$\boldsymbol{r}_{1D} = z\boldsymbol{e}_z = (0,0,z) \,.$$

$S_{\boldsymbol{G}}$ depends only on G_z, which leads to the Bragg plane.

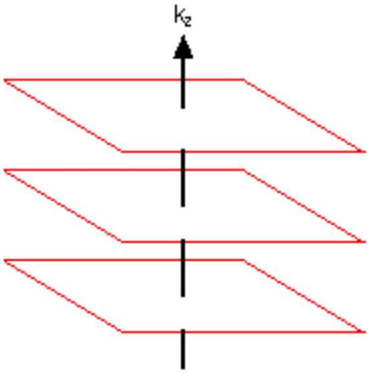


Fig. Bragg plane ($k_z = (2\pi l/a$, l: integer) in the reciprocal lattice space, which is a significant feature common to the 1D system where atoms are arranged along the z axis with a lattice constant a.

18.2 Two dimensional case

The structure factor $S_{\boldsymbol{G}}$ for the 2D case is given by

$$S_{\boldsymbol{G}} = \int n(\boldsymbol{r}_{2D}) e^{-i\boldsymbol{G}\cdot\boldsymbol{r}_{2D}} d\boldsymbol{r}_{2D} = \int\int n(x,y) e^{-i(G_x x+G_y y)} dxdy$$

where

$$\boldsymbol{r}_{2D} = x\boldsymbol{e}_x + y\boldsymbol{e}_y = (x, y, 0),$$

$S_{\boldsymbol{G}}$ depends only on G_x and G_y, which leads to the Bragg ridge (or Bragg rod. or reciprocal rod).

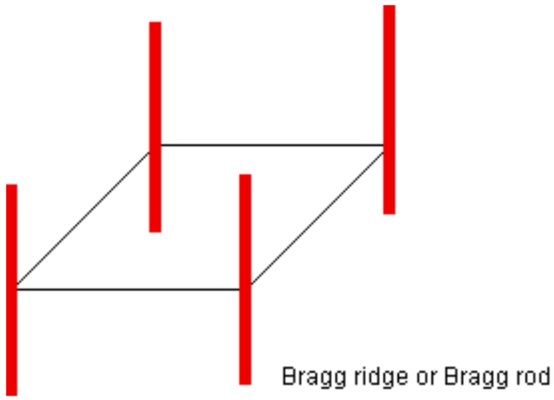


Fig. Bragg ridge (or rod) in the reciprocal lattice space (in the case of square lattice), which is a significant feature common to the 2D system (see "electron diffraction")

18.3 Three dimensional case

The structure factor $S_{\boldsymbol{G}}$ for the 3D case is given by

$$S_{\boldsymbol{G}} = \int n(\boldsymbol{r}_{3D}) e^{-i\boldsymbol{G}\cdot\boldsymbol{r}_{3D}} d\boldsymbol{r}_{3D} = \int\int\int n(x,y,z) e^{-i(G_x x+G_y y+)} dxdy\, dz$$

where

$$\boldsymbol{r}_{3D} = x\boldsymbol{e}_x + y\boldsymbol{e}_y + z\boldsymbol{e}_z = (x, y, z),$$

S_G depends only on G_x, G_y, and G_z, which leads to the Bragg point.

19. Diffraction conditions

19.1 Scattering amplitude

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

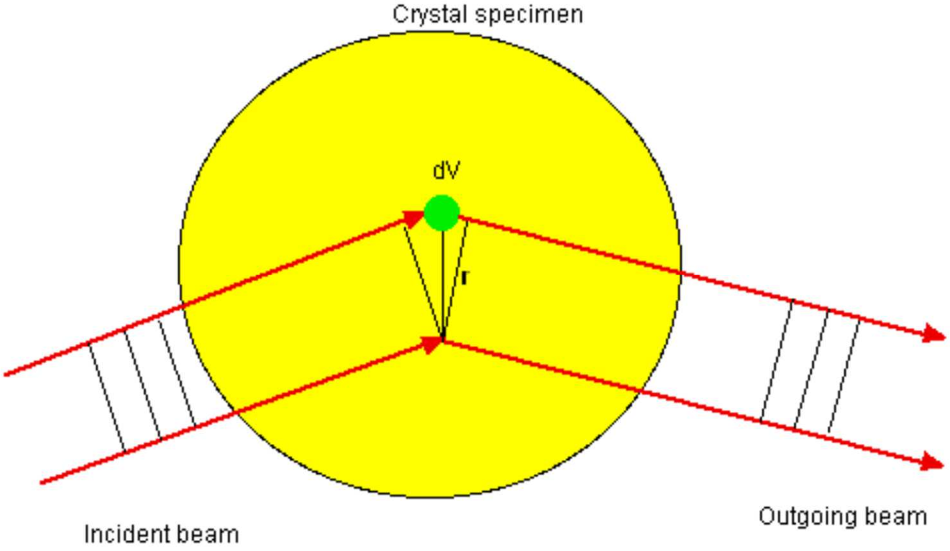


Fig. Geometry of the x-ray scattering.

$\boldsymbol{k}_i = \boldsymbol{k}$, is the incident wavevector.
$\boldsymbol{k}_f = \boldsymbol{k}'$ is the outgoing wavevector.

The difference in phase factor is $\exp[i(\boldsymbol{k}-\boldsymbol{k}')\cdot\boldsymbol{r}]$ between beams scattered from volume elements $\boldsymbol{r}$ apart. The amplitude of the wave scattered from a volume element is proportional to the local electron concentration $n(\boldsymbol{r})$.

The scattering amplitude F is

$$F = \int d\boldsymbol{r} n(\boldsymbol{r}) e^{i(\boldsymbol{k}-\boldsymbol{k}')\cdot\boldsymbol{r}} = \int d\boldsymbol{r} e^{-i\boldsymbol{Q}\cdot\boldsymbol{r}} \sum_{\boldsymbol{G}} n_G e^{i\boldsymbol{G}\cdot\boldsymbol{r}},$$

where $\boldsymbol{Q}$ is the scattering vector

$$\boldsymbol{Q} = \boldsymbol{k}' - \boldsymbol{k}.$$

Then F is rewritten as

$$F = \sum_{\boldsymbol{G}} n_G \int d\boldsymbol{r} e^{i(\boldsymbol{G}-\boldsymbol{Q})\cdot\boldsymbol{r}}.$$

From theses we have

$F = n_G V$ for $\boldsymbol{Q} = \boldsymbol{k}' - \boldsymbol{k} = \boldsymbol{G}$,

and

$F = 0$ otherwise.

This is a Bragg's law.

In elastic scattering (energy is conserved), $|\mathbf{k}'| = |\mathbf{k}|$. Then we have

$$\boldsymbol{k}'^2 = (\boldsymbol{k}+\boldsymbol{G})^2 = \boldsymbol{k}^2 + \boldsymbol{G}^2 + 2\boldsymbol{k}\cdot\boldsymbol{G}$$

or

$2\boldsymbol{k}\cdot\boldsymbol{G} = -\boldsymbol{G}^2$, or $(\boldsymbol{k} + \frac{\boldsymbol{G}}{2})\cdot\frac{\boldsymbol{G}}{2} = 0$

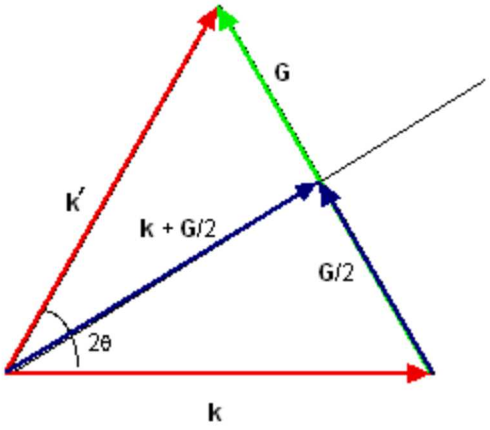


Fig. Geometry of ***k***, ***k′***, and reciprocal lattice vector ***G***.

The vector (***k***+***G***/2) is always perpendicular to the vector ***G***/2.

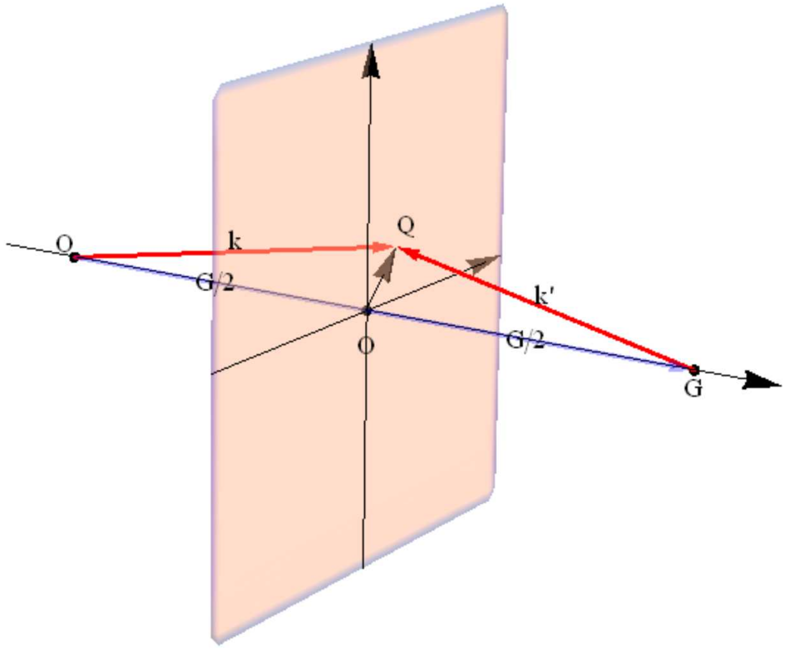


Fig. The Brillouin zone for the 3D reciprocal lattice space. $\boldsymbol{k} = \boldsymbol{k}' + \boldsymbol{G}$.

19.2 Brillouin zone

If $\boldsymbol{G}$ is a reciprocal lattice vector, so is $-\boldsymbol{G}$. With this substitution, we have

$$\boldsymbol{k} - \boldsymbol{k}' = \boldsymbol{G}$$

and

$$(\boldsymbol{k} - \boldsymbol{G}/2) \cdot \boldsymbol{G}/2 = 0 \ .$$

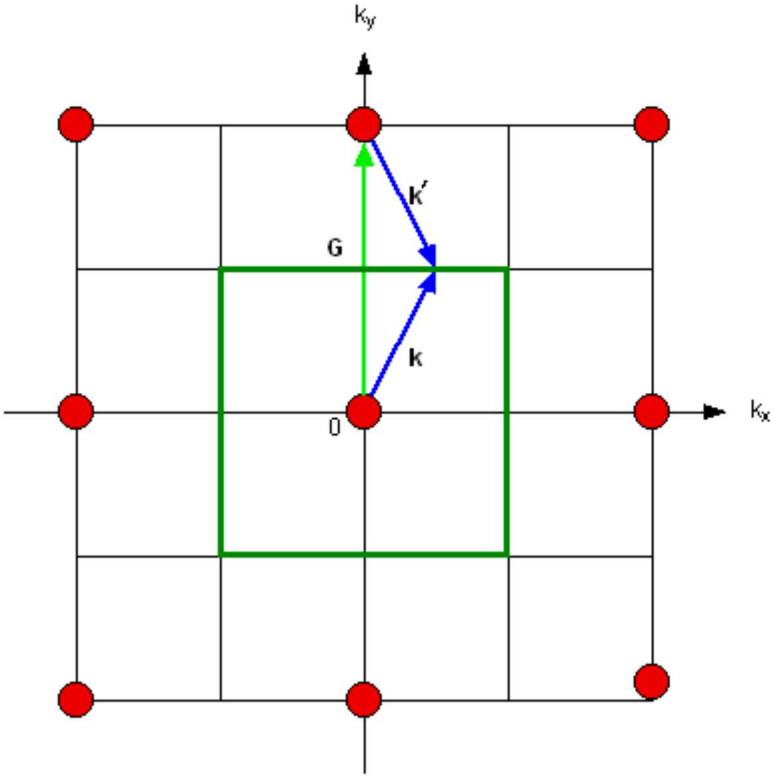


Fig. Condition for the Bragg reflection. It is required that the wavevector ***k*** is located at the zone boundary of the first Brillouin zone in the reciprocal lattice plane. When ***k*** is not on the zone boundary, no Bragg reflection occurs.

We construct a plane normal to ***G*** at its midpoint. This plane forms a part of the zone boundary. A x-ray beam will be diffracted if its wavevector ***k*** has the magnitude and direction required by

$$2\boldsymbol{k} \cdot \boldsymbol{G} = \boldsymbol{G}^2 .$$

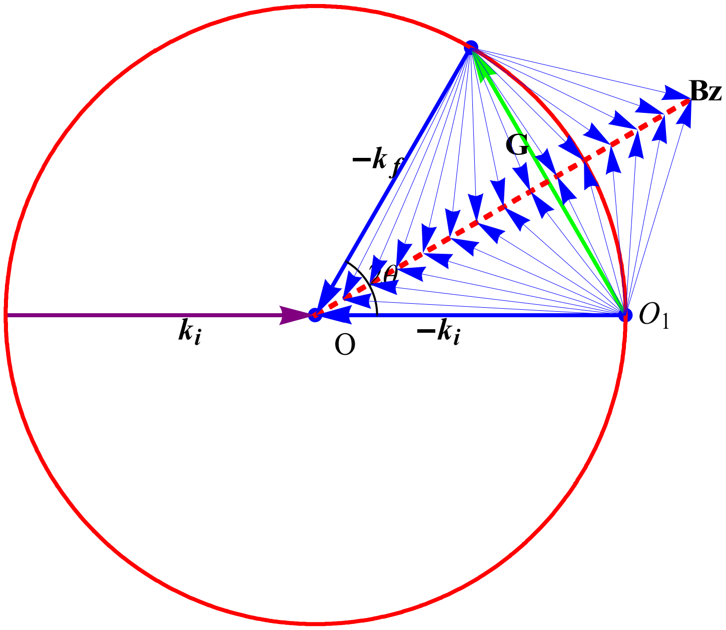
The diffracted beam will then be in the direction $\boldsymbol{k}' = \boldsymbol{k} - \boldsymbol{G}$.

The set of planes that are the perpendicular bisectors of ***G*** is of general importance in the theory of wave propagation in crystals. The first Brillouin zone is the smallest volume entirely enclosed by planes that are perpendicular bisectors of the reciprocal lattice vectors drawn from the origin.

(1) The Brillouin zone exhibits all wavevector (-ki), which can be Bragg reflected by a crystal.

(2) A Brillouin zone is defined as a Wigner-Seitz primitive cell in the reciprocal lattice.

(3) A wave whose wavevector drawn from the origin terminates on any of these planes will satisfy the condition of diffraction: x-ray, phonon, magnon, and electron.



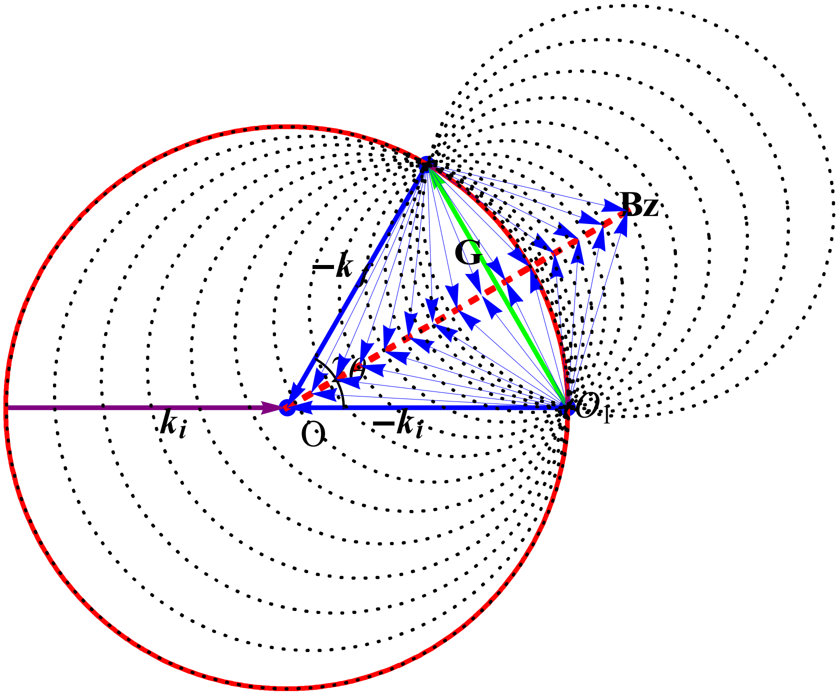


Fig. When the Bragg reflection ($\boldsymbol{G} = \boldsymbol{k}_f - \boldsymbol{k}_i = \boldsymbol{k}' - \boldsymbol{k}$) occurs, the wave vector ($-\boldsymbol{k}_i$) always lies on the Brillouin zone (Bz). $\boldsymbol{k}_f$ ($= \boldsymbol{G} + \boldsymbol{k}_i$) is the wavevector of the outgoing wave

(a) Brillouun zone for square lattice with the unit cell of *a* x *a*

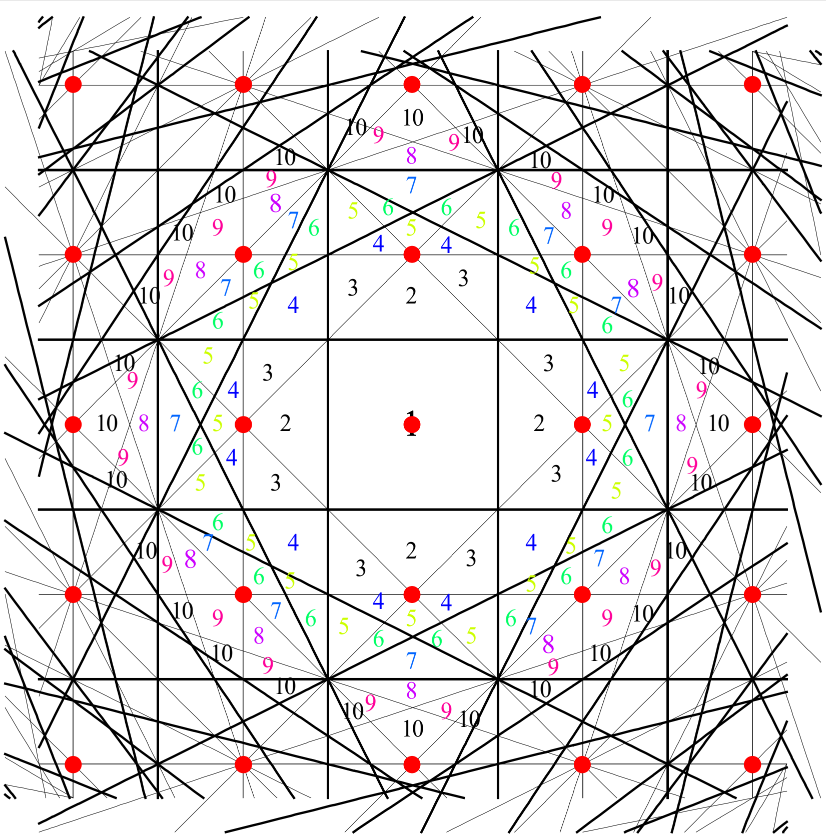


Fig. 2D Brillouin zone for the square lattice. The number denotes the Brillouin zone number.

(b) Brillouin zone for the triangular lattice

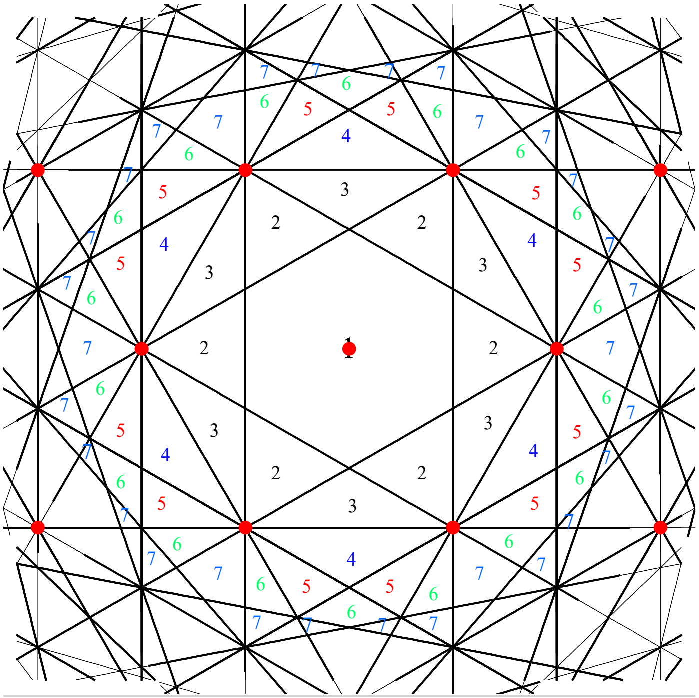


Fig. Brillouin zone for the 2D triangular lattice.

19.3 One dimensional case

We now consider the 1D case of the Brillouin zone. The Bragg condition occurs when $k - k' = 2\pi/a$.

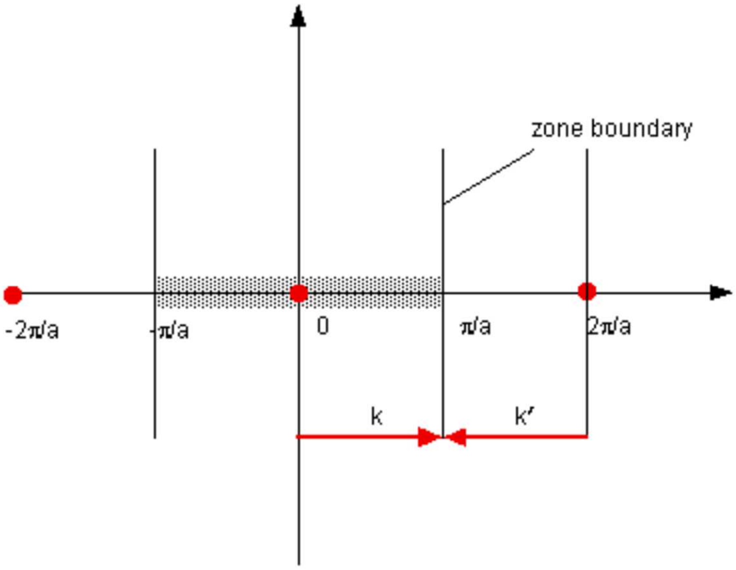


Fig.58 First Brillouin zone for the 1D system with a lattice constant a. Bragg reflection occurs only at $k = \pi/a$.

20. Ewald sphere and scattering

20.1 Construction of Ewald sphere

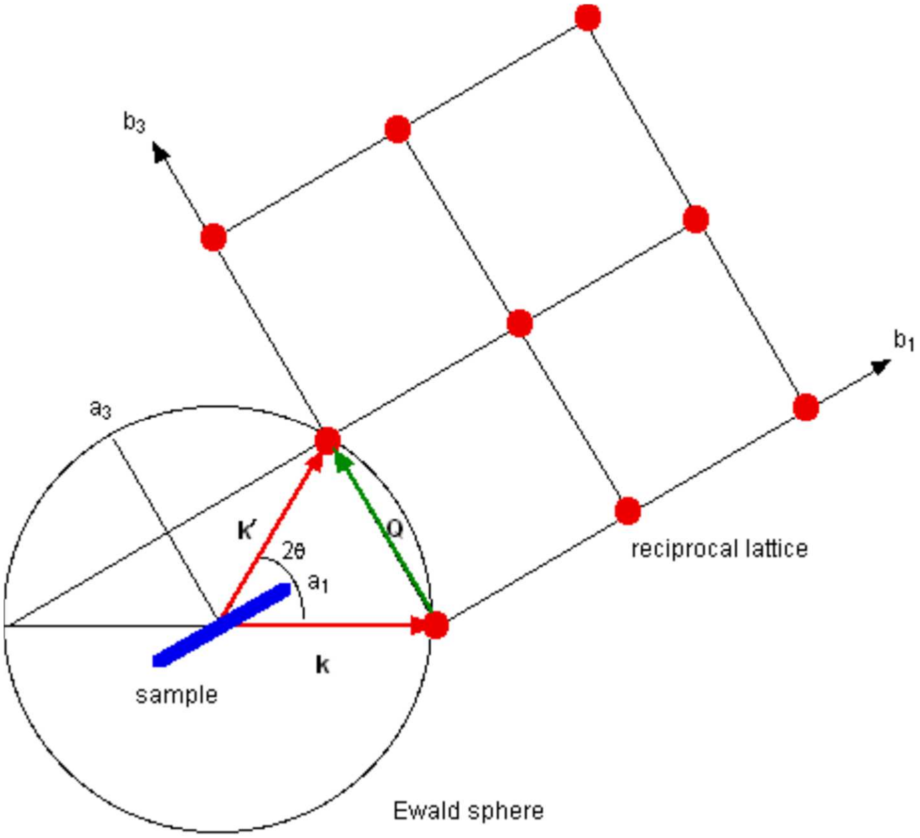


Fig. Ewald sphere. The origin of the reciprocal lattice is located at the end of the wavevector ***k*** of the incident beam.

We draw a sphere of radius $k=2\pi/\lambda$ about the starting point of ***k***. The origin of the reciprocal lattice plane corresponding to the real space of the sample is at the end point of ***k***. A diffracted beam will be formed if this sphere intersects any other point in the reciprocal lattice. The Ewald sphere intercepts a point connected with the end of ***k*** by a reciprocal lattice vector ***G***. This construction is due to Paul Peter Ewald.

Paul Peter Ewald: He was born in Berlin Germany on January 23, 1888. He was a U.S. (German-born) crystallographer and physicist. He was a pioneer of the x-ray diffraction methods. He was also the eponym of Ewald construction and the Ewald sphere. He was a Professor of Physics Department, Brooklyn Polytechnic Institute (1949 – 1959), New York.

He was the father-in-law of Prof. Hans Bethe (the late). He died at Ithaca, New York on August 22, 1985. He was awarded the Max Planck medal in 1978.

20.2 Experimental configuration

Ω is the angle of sample
2θ is the angle between the direction of the incident x-ray and the outgoing x-ray.

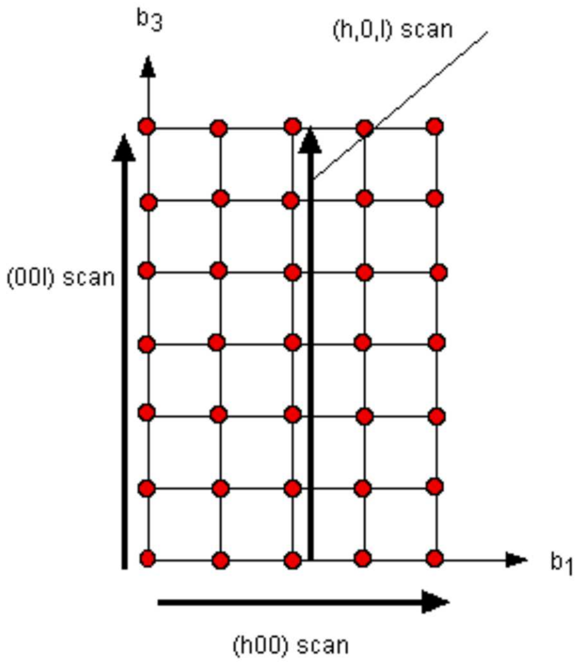


Fig. Schematic diagram of (*hkl*) scan for the x-ray scattering experiment.

20.2.1. (00l) scattering

Ω (= θ) -2θ scan

Ewald sphere-1 (θ-2θ scan)

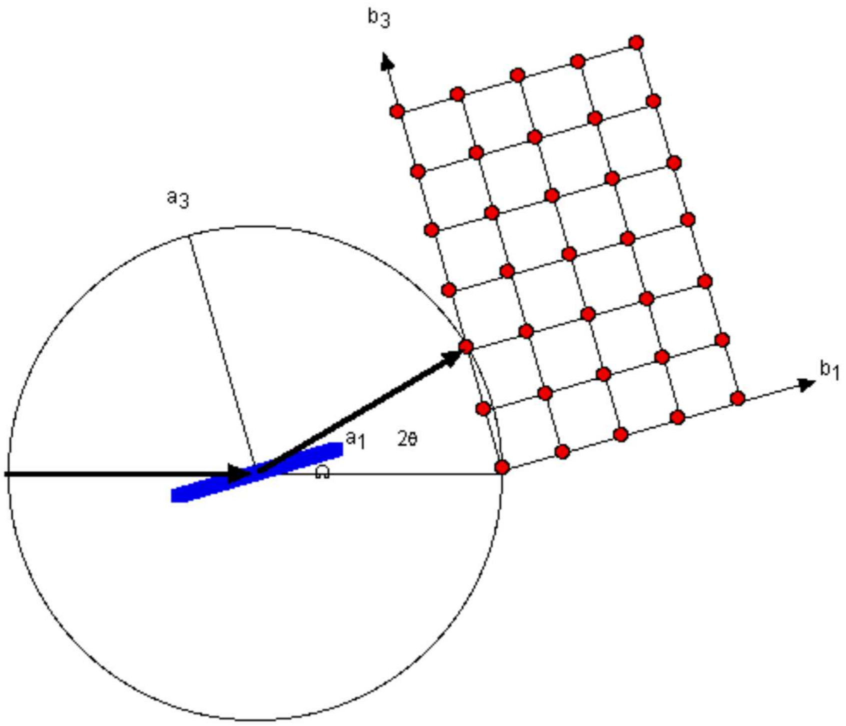


Fig.

Ewald sphere-2 (θ-2θ scan)

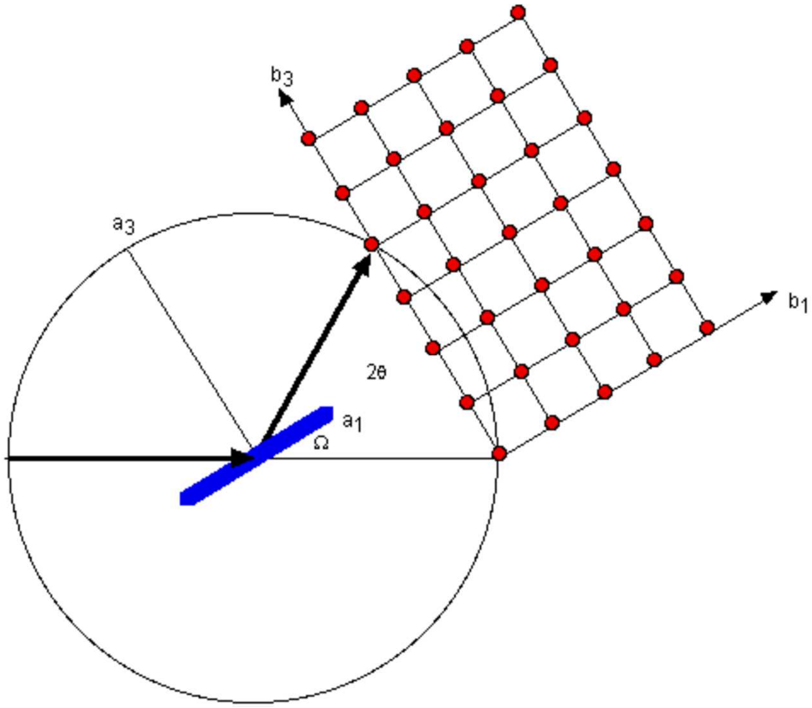
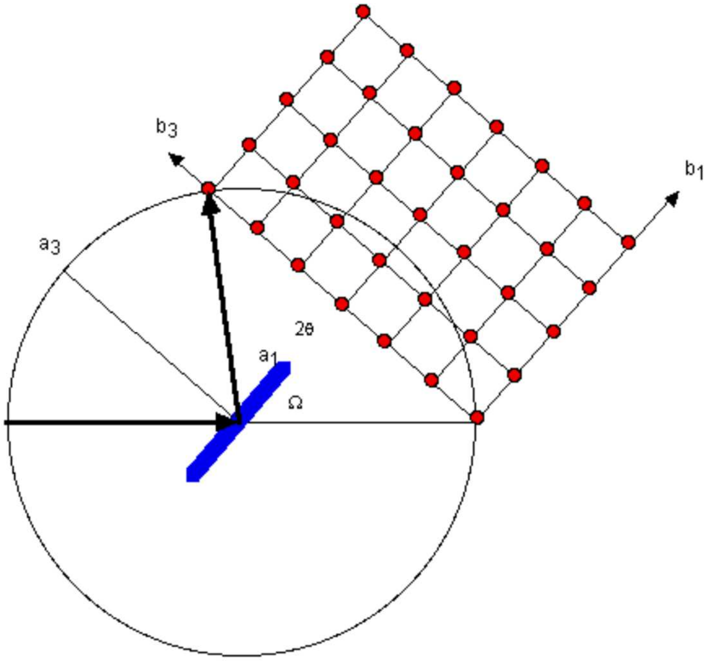


Fig.

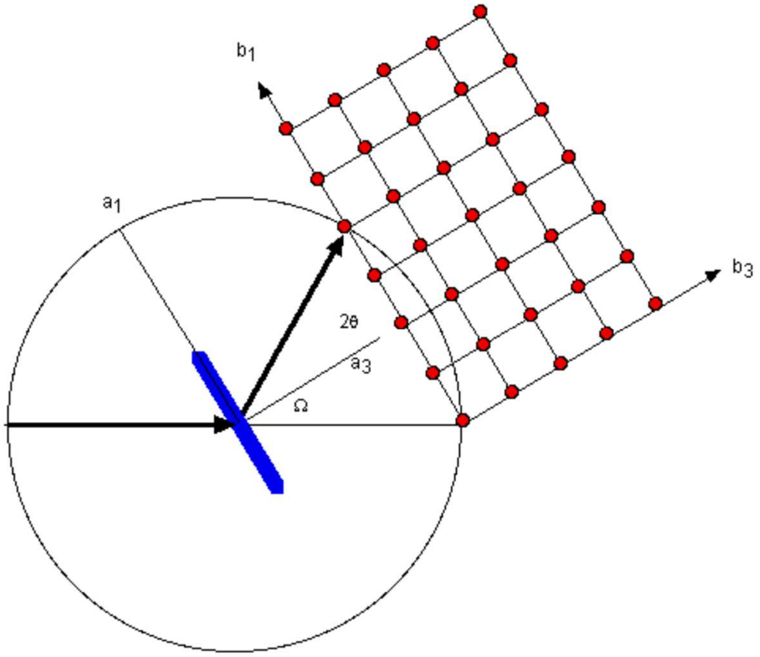
Ewald sphere-3 (θ-2θ scan)



Figs. Examples for the Ewald construction for the (00*L*) x-ray diffraction. Ω (= θ) – 2θ scan.

20.2.2 In-plane (*h, k*,0) scattering

Ω=(90º +θ) - 2θ scan



Figs. Example for the Ewald construction for the (H00) x-ray diffraction. Ω (= θ +90º) – 2θ scan.

20.2.3 Rocking curve around (00*l*) Bragg point.

2θ is fixed, while Ω is rotated.

Note that $Q = \dfrac{4\pi}{\lambda}\sin\theta = const$

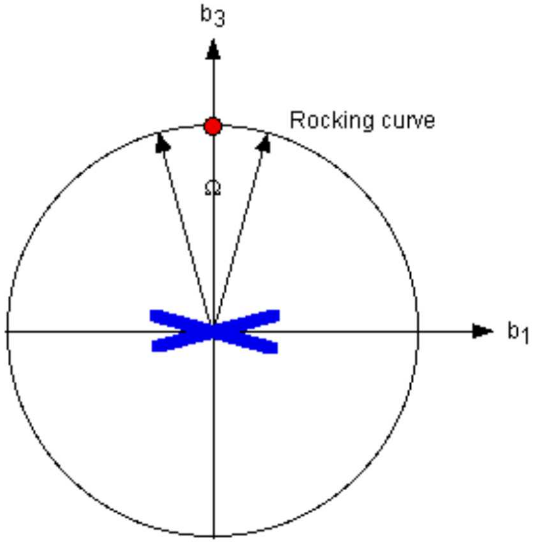


Fig. Schematic diagram of the reciprocal plane for the rocking curve experiment.

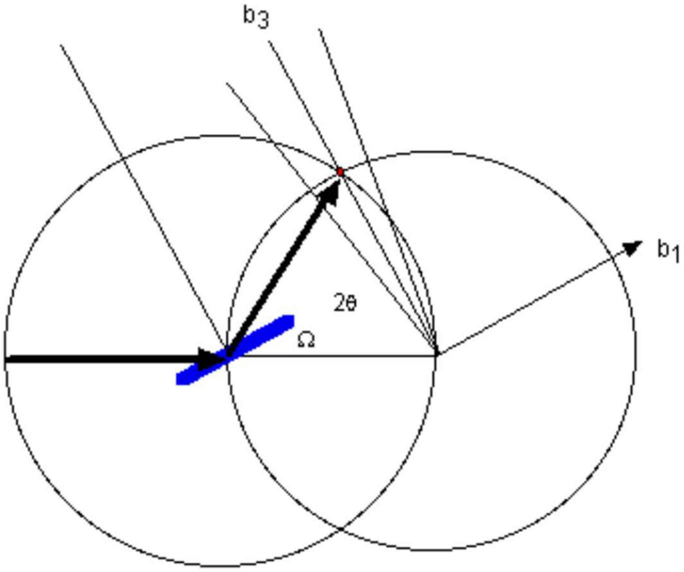


Fig. Example for the Ewald construction for the rocking curve where 2θ = fixed. Ω is rotated.

Using this curve, one can estimate the mosaic spread of the sample.

21. X-ray diffraction in Low dimensional systems

21.1 One dimensional system

For the one dimensional system with the lattice constant *d*, there exist Bragg planes with $k_z = (2\pi/d_c)l$. The Bragg reflections occur on the surface of Ewald sphere where the Bragg planes intersect with the sphere. The incident beam of x-ray is perpendicular to the line of atoms.

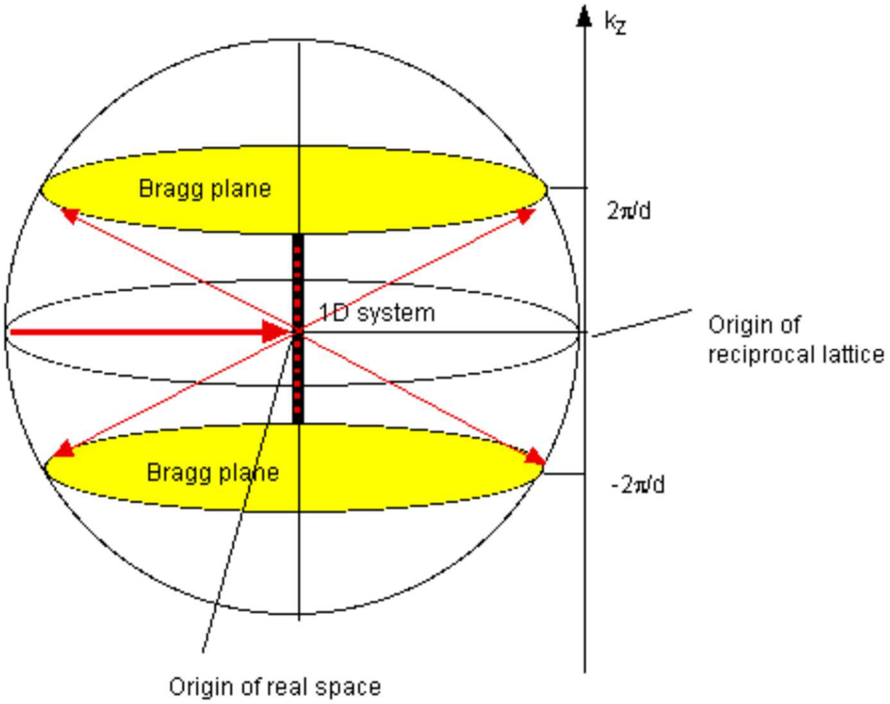


Fig. Schematic diagram of the Ewald construction. Because of the 1D chain, there are Bragg planes in the reciprocal lattice plane. The direction of 1D chain is the same as the direction of incident beam.

The interference condition is

$$k \cos\theta = (2\pi/d)n.$$

Since $k = 2\pi/\lambda$, this is rewritten as $(2\pi/\lambda) \cos\theta = (2\pi/d)n$. or $d \cos\theta = n\lambda$, where d is the lattice constant of the 1D system.

We also consider the case when the incident beam of x-ray is parallel to the line of atoms. We note that a 1D system has Bragg planes in the reciprocal lattice. The direction of diffracted beam is determined using the Ewald sphere.

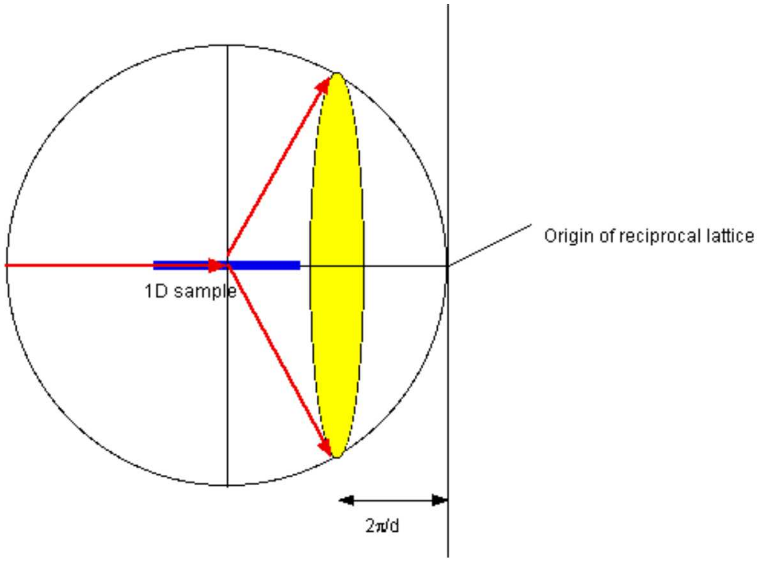


Fig. Schematic diagram of the Ewald construction. Because of the 1D chain, there are Bragg planes in the reciprocal lattice plane. The direction of 1D chain is perpendicular to the direction of incident beam.

The interference condition is

$$k\,(1-\cos\theta)= (2\pi/d)n.$$

Since $k = 2\pi/\lambda$, this is rewritten as $(2\pi/\lambda)\ 2\sin^2(\theta/2) = (2\pi/a)n$.

or

$$2\sin^2(\frac{\theta}{2}) = \frac{\lambda}{d}n\,.$$

21.2 Two dimensional system

A single plane of atoms form a square lattice of lattice constant a. The plane is normal to the incident beam. There exist Bragg rods (Bragg ridge, reciprocal rod). The Bragg reflections occur on the surface of Ewald sphere where the Bragg rods intersect with the sphere.

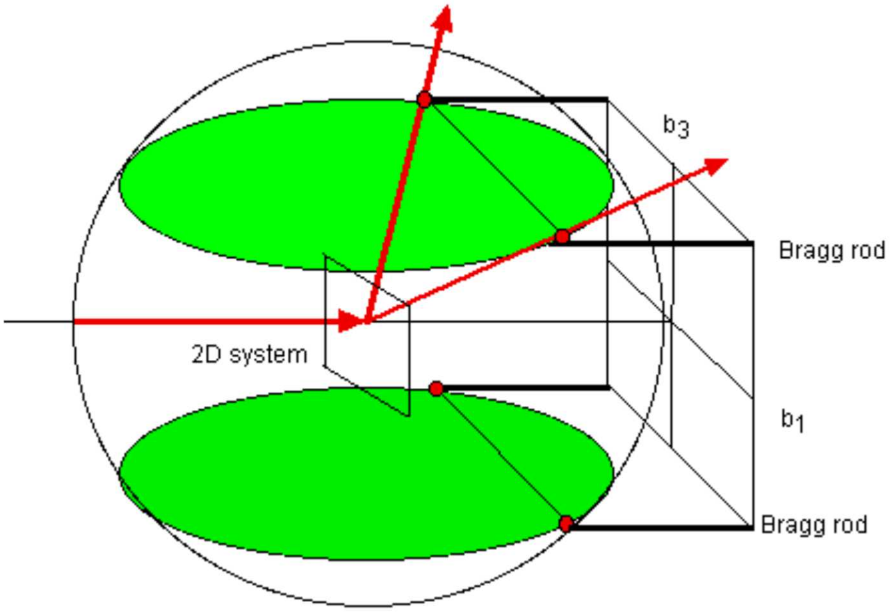


Fig. Schematic diagram of the Ewald construction. Because of the 2D system, there are Bragg rods (ridges) in the reciprocal lattice space. The direction of 2D plane is perpendicular to the direction of incident beam.

21.3 Relation between the lattice and reciprocal lattice for the 2D square and hexagonal lattice

For the square lattice, the shape of the lattice and the reciprocal lattice is the same. The rotation angle between these two lattices is equal to 0º.

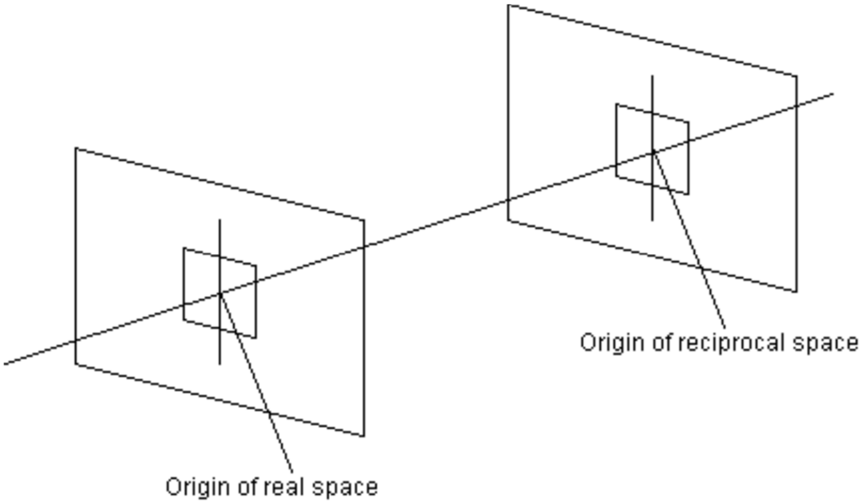


Fig. Relation of the real space and the reciprocal space for the 2D square lattice. The rotation angle between the a_1 axis and b_1 axis is 0º.

For the hexadonal lattice, the shape of the lattice and the reciprocal lattice is the same. The rotation angle between these two lattices is equal to 30º.

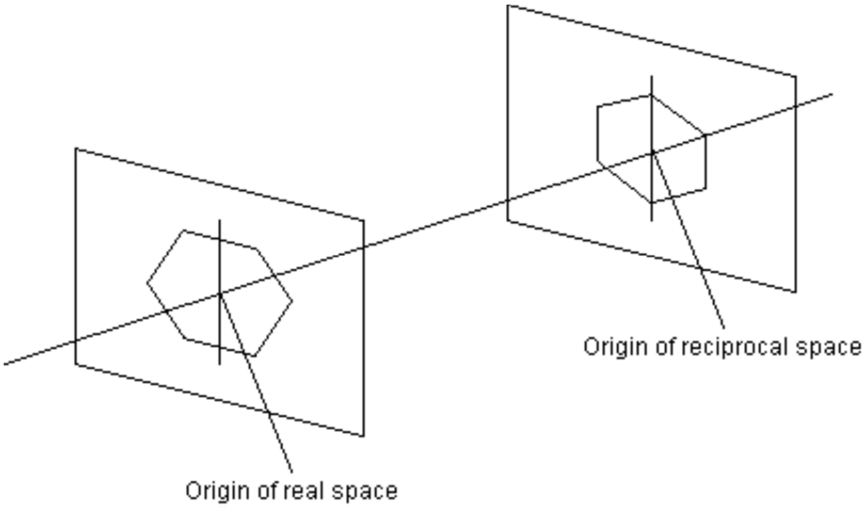


Fig. Relation of the real space and the reciprocal space for the 2D triangular (hexagonal) lattice. The rotation angle between the a_1 axis and b_1 axis is 30º.

22. Debye-Scherrer powder method

In the powdered method, the incident x-ray beam strikes a finely powdered polycrystalline sample contained in a thin-walled capillary tube. The distribution of crystallite orientations will be nearly continuous. Diffracted x-rays leave sample along the generators of cones concentric with the original incident beam. The generators make an angle 2q with the direction of the incident beam. The cones intercept the x-ray film in a series of concentric rings.

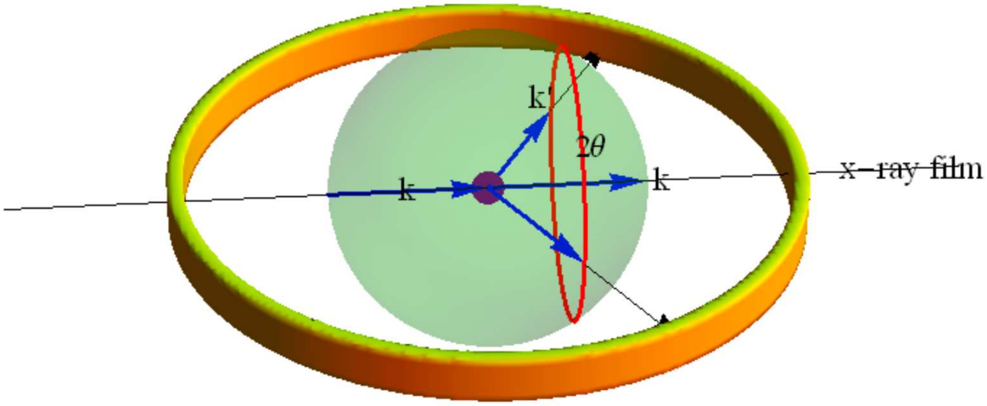


Fig. Schematic diagram for the Debye-Schrerrer powder method. Ewald sphere is also drawn. The outgoing x-ray beam intercepts the x-ray film (ring shape).

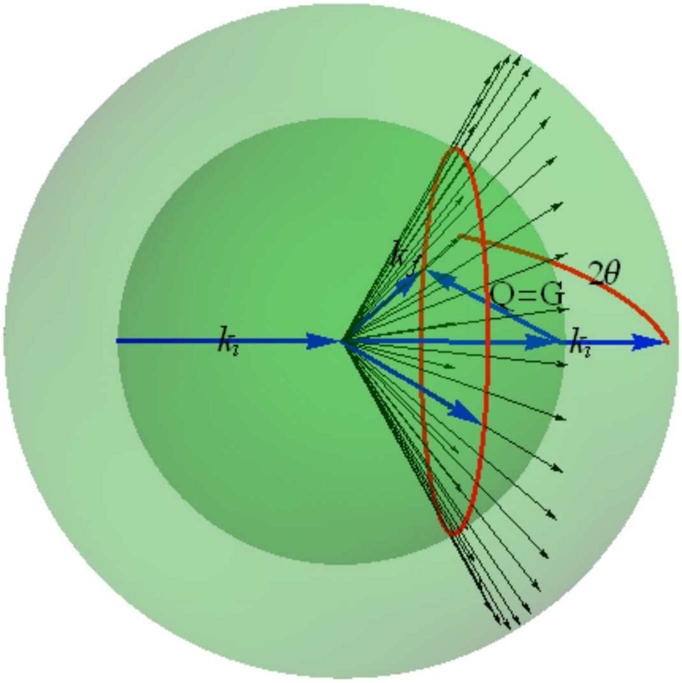


Fig. Construction of the Ewald sphere with $|\boldsymbol{k}|=|\boldsymbol{k}'|= 2\pi/\lambda$. $Q = \boldsymbol{k}' - \boldsymbol{k} = \boldsymbol{G}$ (Bragg condition).

Bragg condition for the x-ray powder diffraction,

$$|\boldsymbol{Q}| = |\boldsymbol{G}| = \frac{4\pi}{\lambda}\sin\theta\,,$$

with

$$\boldsymbol{G} = \boldsymbol{G}(hkl) = h\boldsymbol{b}_1 + k\boldsymbol{b}_2 + l\boldsymbol{b}_3\,.$$

If (*hkl*) are the smallest three integers, we have

$$|\boldsymbol{G}(hkl)| = \frac{2\pi}{d(hkl)}$$

where $d(hkl)$ is the shortest distance between adjacent (*hkl*) planes.

(a) Selection rule for the sc

$$\frac{4\pi}{\lambda}\sin\theta = |\boldsymbol{G}| = \frac{2\pi}{a}\sqrt{g_x^{\ 2} + g_y^{\ 2} + g_z^{\ 2}}$$

where

$$\boldsymbol{G} = g_x\boldsymbol{b}_x + g_y\boldsymbol{b}_y + g_z\boldsymbol{b}_x = \frac{2\pi}{a}(g_x, g_y, g_z)$$

where g_x, g_y, and g_z are integers. For the sc structure, it is required that

$g_x^{\ 2} + g_y^{\ 2} + g_z^{\ 2} =$ 1, 2, 3, 4, 5, 6, 8, 9, 10, 11, 12, 13, 14, 16, 17, 18, 19, 20, 21, 22, 24, 25, 26, 27, 29, 30, 32, ...

(b) Selection rule for the fcc

$$\frac{4\pi}{\lambda}\sin\theta = |\boldsymbol{G}| = \frac{2\pi}{a}\sqrt{g_x^{\ 2} + g_y^{\ 2} + g_z^{\ 2}}$$

The reciprocal lattice vector is given by

$$\boldsymbol{G} = g_x\boldsymbol{b}_x + g_y\boldsymbol{b}_y + g_z\boldsymbol{b}_x = \frac{2\pi}{a}(g_x, g_y, g_z),$$

with

$$\begin{aligned} g_x &= -g_1 + g_2 + g_3 \\ g_y &= g_1 - g_2 + g_3 \\ g_z &= g_1 + g_2 - g_3 \end{aligned}$$

where g_1, g_2, g_3 are integers. There are relations between (g_x, g_y, g_z) and (g_1, g_2, g_3). Note that all indices of (g_x, g_y, g_z) are odd or even. There is a selection rule for the indices (g_x, g_y, g_z).

g_x	g_y	g_z	g_1	g_2	g_3
1	1	1	1	1	1
2	0	0	0	1	1
2	2	0	1	1	2
3	1	1	1	2	2

2	2	2	2	2	2
4	0	0	0	2	2
3	3	1	2	2	3
4	2	0	1	2	3
4	2	2	2	3	3
5	1	1	1	3	3

Selection rule for the indices (g_x, g_y, g_z) for the fcc.

For fcc structure, it is required that

$$g_x^2 + g_y^2 + g_z^2 = 3, 4, 8, 11, 12, 16, 19, 20, 24, 27, 32, 35, 40, 36, 43, 44, 48 \quad \text{(fcc)}$$

(c) Selection rule for the bcc

$$\frac{4\pi}{\lambda}\sin\theta = |\boldsymbol{G}| = \frac{2\pi}{a}\sqrt{g_x^2 + g_y^2 + g_z^2}\ .$$

The reciprocal lattice vector is given by

$$\boldsymbol{G} = g_x\boldsymbol{b}_x + g_y\boldsymbol{b}_y + g_z\boldsymbol{b}_x = \frac{2\pi}{a}(g_x, g_y, g_z)$$

with

$$g_x = g_2 + g_3$$
$$g_y = g_1 + g_3$$
$$g_z = g_1 + g_2$$

where g_1, g_2, g_3 are integers. There are relations between (g_x, g_y, g_z) and (g_1, g_2, g_3). Note that

$$g_x + g_y + g_z = 2(g_1 + g_2 + g_3)$$

which is even.

g_x	g_y	g_z	g_1	g_2	g_3
1	1	0	0	0	1
2	0	0	-1	1	1
2	1	1	0	1	1

2	2	0	0	0	2
3	1	0	-1	1	2
2	2	2	1	1	1
3	2	1	0	1	2
4	0	0	-2	2	2

Selection rule for the indices (g_x, g_y, g_z) for the bcc

For bcc structure, it is required that

$$g_x{}^2 + g_y{}^2 + g_z{}^2 = 2, 4, 6, 8, 10, 12, 14, 16, 18, 20, 22, 24, \ldots.. \text{ (bcc)}$$

23. Structure factor calculations of KCl and KBr (NaCl type structure)

In KCl, the numbers of electrons of K^+ (18 electrons) and Cl^- ions are equal (18 electrons)

$$f(K^+) \approx f(Cl^-).$$

K+	(1/2, 0, 0), (0,1/2,0), (0, 0, 1/2), (1/2, 1/2, 1/2)
Cl^-	(0, 0, 0), (0,1/2,1/2), (1/2, 0, 1/2), (1/2, 1/2, 0).

The crystal looks to x-rays as if it were a monatomic simple cubic lattice with a lattice constant *a*/2.

$$S_G(v_1, v_2, v_3) = f_{Cl}[1 + e^{-i\pi(v_2+v_3)} + e^{-i\pi(v_3+v_1)} + e^{-i\pi(v_1+v_2)}]$$
$$+ f_K[e^{-i\pi v_1} + e^{-i\pi v_2} + e^{-i\pi v_3} + e^{-i\pi(v_1+v_2+v_3)}]$$

where $g_x = v_1$, $gy = v_2$, and $g_z = v_3$.

g_x	g_y	g_z	$S_G(v_1, v_2, v_3)$
1	1	1	$4(-f_K+f_{Cl}) = 0$
2	0	0	$4(f_K+f_{Cl})$
2	2	0	$4(f_K+f_{Cl})$
3	1	1	$4(-f_K+f_{Cl}) = 0$
2	2	2	$4(f_K+f_{Cl})$
4	0	0	$4(f_K+f_{Cl})$
3	3	1	$4(-f_K+f_{Cl}) = 0$
4	2	0	$4(f_K+f_{Cl})$

In KBr, the form factor of Br$^-$ (36 electrons) is quite different from that of K$^+$ (18 electrons)

g_x	g_y	g_z	$S_G(v_1,v_2,v_3)$
1	1	1	$4(-f_K+f_{Br})$
2	0	0	$4(f_K+f_{Br})$
2	2	0	$4(f_K+f_{Br})$
3	1	1	$4(-f_K+f_{Br})$
2	2	2	$4(f_K+f_{Br})$
4	0	0	$4(f_K+f_{Br})$
3	3	1	$4(-f_K+f_{Br})$
4	2	0	$4(f_K+f_{Br})$

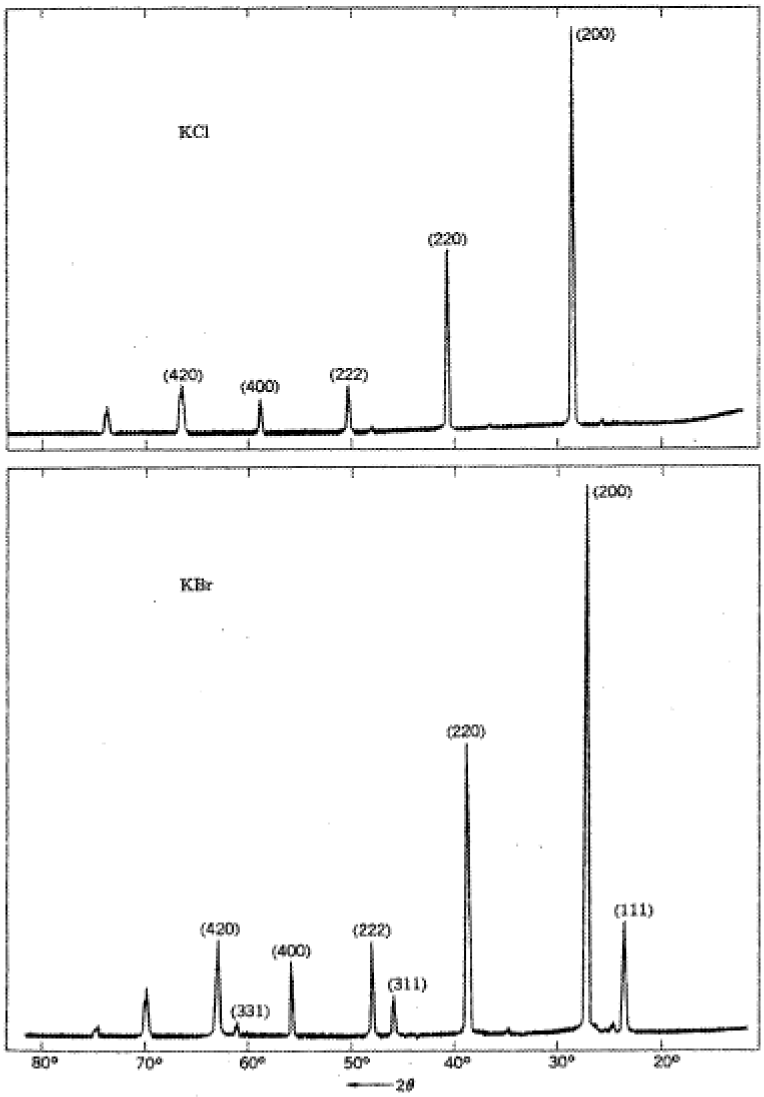


Fig.74 Comparison of x-ray reflections from KCl and KBr powers. (Kittel, ISSP 4th edition, Fig.31, p. 81)

APPENDIX-I Form factor of 1D x-ray diffraction

For simplicity, we consider the electron number density *N*(*x*) with a period *a* in the *x* direction (one dimensional case).

$$N(x) = N(x+a) .$$

Then *N*(*x*) may be expressed in terms of the Fourier series.

$$\begin{aligned}
N(x) &= \frac{b_0}{2} + \sum_{n=1}^{\infty}\{a_n \sin(n\frac{2\pi}{a}x) + b_n \cos(n\frac{2\pi}{a}x)\} \\
&= \frac{b_0}{2} + \sum_{n=1}^{\infty}[\frac{a_n}{2i}\{\exp(i\frac{2\pi n}{a}x) - \exp(-i\frac{2\pi n}{a}x)\} + \frac{b_n}{2}\{\exp(i\frac{2\pi n}{a}x) + \exp(-i\frac{2\pi n}{a}x)\}] \\
&= \frac{b_0}{2} + \sum_{n=1}^{\infty}[-i\frac{a_n}{2}\{\exp(i\frac{2\pi n}{a}x) - \exp(-i\frac{2\pi n}{a}x)\} + \frac{b_n}{2}\{\exp(i\frac{2\pi n}{a}x) + \exp(-i\frac{2\pi n}{a}x)\} \\
&= \frac{b_0}{2} + \sum_{n=1}^{\infty}[(-i\frac{a_n}{2} + \frac{b_n}{2})\exp(i\frac{2\pi n}{a}x) + (i\frac{a_n}{2} + \frac{b_n}{2})\exp(-i\frac{2\pi n}{a}x)]
\end{aligned}$$

where

$$b_0 = \frac{2}{a}\int_0^a N(x)dx$$

$$a_n = \frac{2}{a}\int_0^a N(x)\sin(\frac{2\pi n}{a}x)dx$$

$$b_n = \frac{2}{a}\int_0^a N(x)\cos(\frac{2\pi n}{a}x)dx$$

We note that

$$\begin{aligned}
a_{-n} &= -a_n \\
b_{-n} &= b_n \\
a_0 &= 0
\end{aligned}$$

and that

$$(-i\frac{a_{-n}}{2}+\frac{b_{-n}}{2})=i\frac{a_n}{2}+\frac{b_n}{2}$$

Then the expression of $N(x)$ can be rewritten as

$$\begin{aligned} N(x) &= \frac{b_0}{2}+\sum_{n=1}^{\infty}[(-i\frac{a_n}{2}+\frac{b_n}{2})\exp(i\frac{2\pi n}{a}x)+(i\frac{a_n}{2}+\frac{b_n}{2})\exp(-i\frac{2\pi n}{a}x)] \\ &= \sum_{n=-\infty}^{\infty}[(-i\frac{a_n}{2}+\frac{b_n}{2})\exp(i\frac{2\pi n}{a}x)] \end{aligned}$$

where

$$\begin{aligned} g_n &= \frac{2\pi n}{a} \\ N_n &= -i\frac{a_n}{2}+\frac{b_n}{2}=\frac{1}{a}\int_0^a N(x)\exp(i\frac{2\pi n}{a}x)dx \\ N_{-n} &= N_n^{\ *} \\ N_0 &= -i\frac{a_0}{2}+\frac{b_0}{2}=\frac{b_0}{2} \end{aligned}$$

For simplicity we use the notation

$$N(x)=\sum_g N_g\exp(igx)$$

where

$$\begin{aligned} N_n &= N_g \\ g_n &= g \end{aligned}$$

The electron number density satisfies the periodic condition,

$$N(x+a)=\sum_g N_g\exp[ig(x+a)]=\exp(iga)\sum_g N_g\exp(igx)=\exp(iga)N(x)=N(x)$$

where

$$\exp(iga)=\exp(i\frac{2\pi n}{a}a)=1$$

Thus we have

$$N(x) = \sum_g N_g \exp(igx)$$

with

$$N_g = \frac{1}{a}\int_0^a dx N(x) e^{-igx}$$

APPENDIX-II Poisson summation formula

(a) Poisson summataion formula

For appropriate functions $f(x)$, the Poisson summation formula may be stated as

$$\sum_{n=-\infty}^{\infty} f(x=n) = \sqrt{2\pi}\sum_{m=-\infty}^{\infty} F(k=m), \tag{1}$$

where m and n are integers, and $F(k)$ is the Fourier transform of the function $f(x)$ and is defined by

$$F(k) = \boldsymbol{F}[f(x)] = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} e^{-ikx} f(x)dx\,.$$

Note that the inverse Fourier transform is given by

$$f(x) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} e^{ikx} F(k)dk\,.$$

The factor of the right hand side of Eq.(1) arises from the definition of the Fourier transform.

((**Proof**)) The proof of Eq.(1) is given as follows.

From the definition of the Fourier transform, we have

$$f(x=n) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} e^{ikn} F(k)dk = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} F(k)dk e^{ikn}$$

and

$$\sum_{n=-\infty}^{\infty} f(x=n) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} F(k)dk \sum_{n=-\infty}^{\infty} e^{ikn} \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} F(k)dk I(k)$$

We evaluate the factor

$$I(k) = \sum_{n=-\infty}^{\infty} e^{ikn} .$$

It is evident that $I(k)$ is not equal to zero only when $k = 2\pi m$ (m; integer). Therefore $I(k)$ can be expressed by

$$I(k) = A \sum_{m=-\infty}^{\infty} \delta(k - 2\pi m) ,$$

where A is the normalization factor. Then

$$\begin{aligned}
\sum_{n=-\infty}^{\infty} f(x = n) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} F(k)dk[A \sum_{m=-\infty}^{\infty} \delta(k - 2\pi m)] \\
&= \frac{A}{\sqrt{2\pi}} \sum_{m=-\infty}^{\infty} \int_{-\infty}^{\infty} F(k)\delta(k - 2\pi m)dk \\
&= \frac{A}{\sqrt{2\pi}} \sum_{m=-\infty}^{\infty} F(k = 2\pi m) \\
&= \frac{A}{\sqrt{2\pi}} \sum_{n=-\infty}^{\infty} F(k = 2\pi n)
\end{aligned}$$

The normalization factor, A, is readily shown to be 2π by considering the symmetrical case

$$f(x = n) = e^{-\pi n^2} ,$$

$$F(k = 2\pi n) = \frac{1}{\sqrt{2\pi}} e^{-\pi n^2}$$

((**Mathematica**))

```
f[x_] = Exp[-π x^2];
FourierTransform[f[x], x, k,
 FourierParameters → {0, -1}]
```

$$\frac{e^{-\frac{k^2}{4\pi}}}{\sqrt{2\pi}}$$

Since

$$A = \frac{\sqrt{2\pi}\, f(x = n)}{F(k = 2\pi n)} = 2\pi\,.$$

or

$$I(k) = \sum_{n=-\infty}^{\infty} e^{ikn} = 2\pi \sum_{m=-\infty}^{\infty} \delta(k - 2\pi m)\,. \qquad (2)$$

Using this formula, we have

$$\sum_{n=-\infty}^{\infty} f(x = n) = \sqrt{2\pi} \sum_{n=-\infty}^{\infty} F(k = 2\pi n)\,. \qquad \text{(Poisson sum formula)}$$

(b) Dirac comb

When we put $k = 2\pi x$ in I of Eq.(2)

$$\begin{aligned}\sum_{n=-\infty}^{\infty} e^{2\pi i x n} &= 2\pi \sum_{m=-\infty}^{\infty} \delta(2\pi x - 2\pi m) \\ &= \frac{2\pi}{2\pi} \sum_{m=-\infty}^{\infty} \delta(x - m) \\ &= \sum_{m=-\infty}^{\infty} \delta(x - m)\end{aligned}$$

or

$$\sum_{n=-\infty}^{\infty} e^{2\pi i x n} = \sum_{m=-\infty}^{\infty} \delta(x - m) \qquad \text{(Dirac comb)} \qquad (3)$$

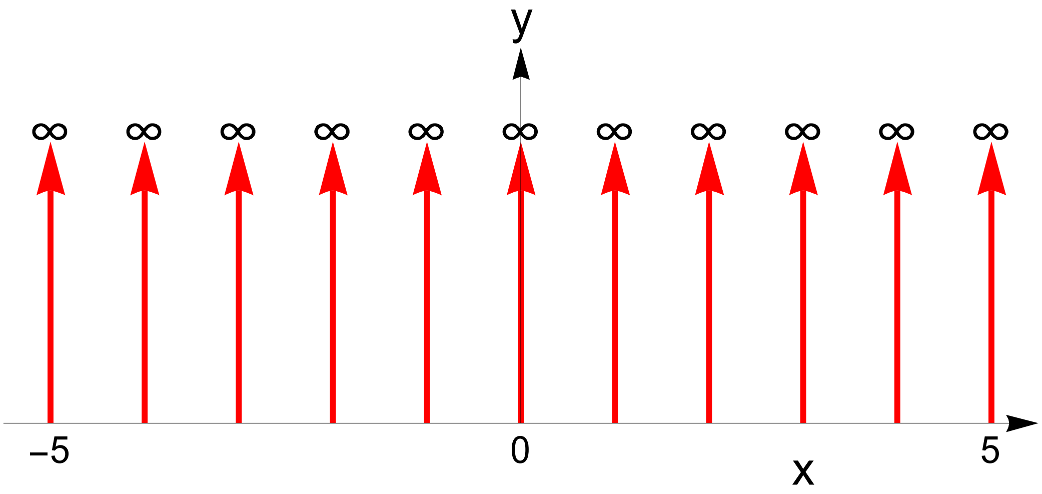


Fig. Plot of the Dirac comb as a function of x: $\sum_{m=-\infty}^{\infty}\delta(x-m)$.

(c) Convolution of Dirac comb: another method in the derivation of Poisson sum formula

The convolution of functions $f(x)$ and $g(x)$ is defined by

$$f*g=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}f(x-\xi)g(\xi)d\xi=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}f(\xi)g(x-\xi)d\xi$$

The Fourier transform of the convolution is given by

$$\boldsymbol{F}[f*g]=\boldsymbol{F}[f]\boldsymbol{F}[g].$$

Here we assume that

$$g(x)=\sum_{n=-\infty}^{\infty}\delta(x-na). \qquad \text{(Dirac comb)}$$

The Fourier transform of $g(x)$ is

$$G(k)=\boldsymbol{F}[g(x)]=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}e^{-ikx}\sum_{n=-\infty}^{\infty}\delta(x-na)dx=\frac{1}{\sqrt{2\pi}}\sum_{n=-\infty}^{\infty}e^{-ikna}.$$

The convolution $f*g$ is obtained as

$$\begin{aligned}f*g&=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}f(x-\xi)\sum_{n=-\infty}^{\infty}\delta(\xi-na)d\xi\\&=\frac{1}{\sqrt{2\pi}}\sum_{n=-\infty}^{\infty}\int_{-\infty}^{\infty}f(x-\xi)\delta(\xi-na)d\xi.\\&=\frac{1}{\sqrt{2\pi}}\sum_{n=-\infty}^{\infty}f(x-na)\end{aligned} \qquad (4)$$

The Fourier transform of the convolution is

$$\boldsymbol{F}[f*g]=F(k)G(k)=\frac{1}{\sqrt{2\pi}}F(k)\sum_{n=-\infty}^{\infty}e^{-ikna}.$$

Here we use the Poisson summation formula;

$$\sum_{n=-\infty}^{\infty} e^{-ikna} = \sum_{n=-\infty}^{\infty} e^{ikna} = \sum_{m=-\infty}^{\infty} \delta(\frac{ka}{2\pi} - m)$$

$$= \sum_{m=-\infty}^{\infty} \delta[\frac{a}{2\pi}(k - \frac{2\pi m}{a})]$$

$$= \frac{2\pi}{|a|} \sum_{m=-\infty}^{\infty} \delta(k - \frac{2\pi m}{a})$$

where $\delta(ax) = \frac{1}{|a|}\delta(x)$, and

$$\sum_{n=-\infty}^{\infty} e^{2\pi ixn} = \sum_{m=-\infty}^{\infty} \delta(x-m), \qquad \text{(Dirac comb)}$$

with $x = \frac{ka}{2\pi}$. Then we get

$$\boldsymbol{F}[f*g] = \frac{1}{\sqrt{2\pi}} F(k) \sum_{n=-\infty}^{\infty} e^{-ikna} = \frac{1}{\sqrt{2\pi}} F(k) \sum_{n=-\infty}^{\infty} e^{ikna}$$

$$= \frac{1}{\sqrt{2\pi}} \frac{2\pi}{|a|} \sum_{m=-\infty}^{\infty} \delta(k - \frac{2\pi m}{a}) F(k)$$

$$= \frac{1}{\sqrt{2\pi}} \frac{2\pi}{|a|} \sum_{m=-\infty}^{\infty} \delta(k - \frac{2\pi m}{a}) F(k = \frac{2\pi m}{a})$$

The inverse Fourier transform of $\boldsymbol{F}[f*g]$ is obtained as

$$f*g = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \boldsymbol{F}[f*g] e^{ikx} dk$$

$$= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{ikx} dk \frac{1}{\sqrt{2\pi}} \frac{2\pi}{|a|} \sum_{m=-\infty}^{\infty} \delta(k - \frac{2\pi m}{a}) F(k = \frac{2\pi m}{a})$$

$$= \left|\frac{1}{a}\right| \sum_{m=-\infty}^{\infty} F(k = \frac{2\pi}{a} m) \int_{-\infty}^{\infty} e^{ikx} dk \delta(k - \frac{2\pi m}{a})$$

$$= \frac{1}{|a|} \sum_{m=-\infty}^{\infty} F(k = \frac{2\pi}{a} m) e^{i\frac{2\pi m}{a}x}$$

where

$$F(k = \frac{2\pi}{a} m) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-i\frac{2\pi}{a}mx} f(x) dx .$$

Finally we get

$$f * g = \frac{1}{\sqrt{2\pi}} \sum_{n=-\infty}^{\infty} f(x - na) = \frac{1}{|a|} \sum_{m=-\infty}^{\infty} F(k = \frac{2\pi m}{a}) e^{i\frac{2\pi m}{a}x} .$$

or

$$\sum_{n=-\infty}^{\infty} f(x - na) = \frac{\sqrt{2\pi}}{|a|} \sum_{m=-\infty}^{\infty} F(k = \frac{2\pi m}{a}) e^{i\frac{2\pi m}{a}x} . \tag{5}$$

When $a = 1$, we get

$$\sum_{n=-\infty}^{\infty} f(x - n) = \sqrt{2\pi} \sum_{m=-\infty}^{\infty} F(k = 2\pi m) e^{i2\pi mx} . \tag{6}$$

When $x = 0$,

$$\sum_{n=-\infty}^{\infty} f(x = n) = \sqrt{2\pi} \sum_{m=-\infty}^{\infty} F(k = 2\pi m) . \tag{7}$$

This is the Poisson sum formula.

(d) Fourier transform of periodic function

We consider a periodic function $N(x)$;

$$N(x + a) = N(x) ,$$

where a is the periodicity. The function $N(x)$ can be described by

$$\begin{aligned} N(x) &= \sum_{n=-\infty}^{\infty} f(x - na) = \frac{\sqrt{2\pi}}{a} \sum_{m=-\infty}^{\infty} F(k = \frac{2\pi m}{a}) e^{i\frac{2\pi m}{a}x} \\ &= \sum_{G} N_G e^{iGx} \end{aligned}$$

where $a>0$. Note that $f(x)$ is defined only in the limited region (for example, $-a/2 \leq x \leq a/2$). G is the reciprocal lattice defined by

$$G = \frac{2\pi}{a} m .$$

The Fourier coefficient N_G is given by

$$
\begin{aligned}
N_G &= \frac{\sqrt{2\pi}}{a} F(k=G) \\
&= \frac{1}{a}\int_{-\infty}^{\infty} e^{-iGx} f(x)dx = \frac{1}{a}\int_{-a/2}^{a/2} e^{-iGx} f(x)dx
\end{aligned}
.
$$

where $f(x)$ is just like a Gaussian distribution function around $x = 0$.

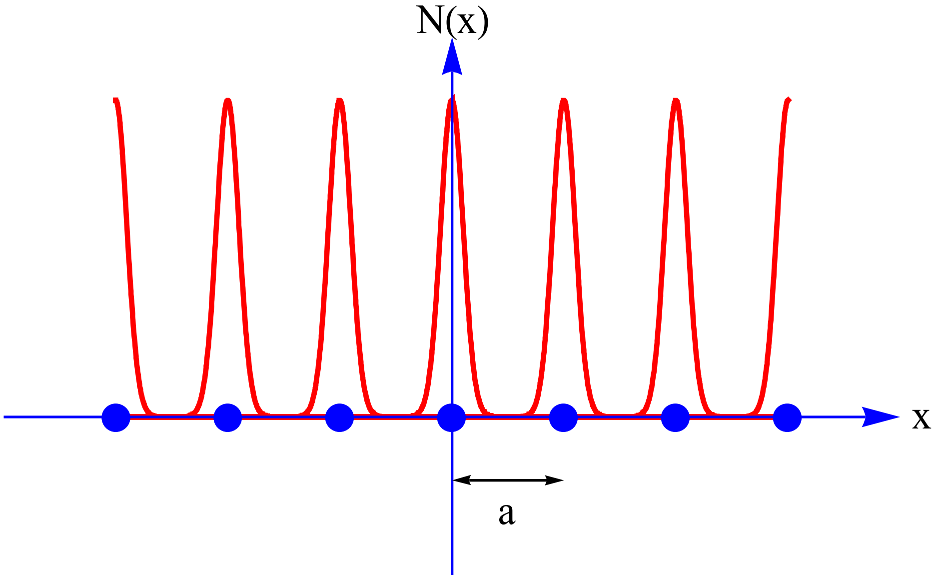


Fig. Plot of $N(x)$ as a function of x. a is the lattice constant of the one-dimensional chain.

((**Example**))

Suppose that $f(x)$ is given by a Gaussian distribution,

$$
f(x) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{x^2}{2\sigma^2}\right).
$$

Then we get

$$
N_G = \frac{1}{a}\int_{-a/2}^{a/2} e^{-iGx} f(x)dx = \frac{1}{2}\exp\left(-\frac{1}{2}G^2\sigma^2\right)\left[erf\left(\frac{1-2iG\sigma^2}{2\sqrt{2}\sigma}\right) + erf\left(\frac{1+2iG\sigma^2}{2\sqrt{2}\sigma}\right)\right],
$$

where erf(x) is the error function and is defined by

$$
erf(z) = \frac{2}{\sqrt{\pi}}\int_0^z e^{-t^2} dt
$$

Figure shows the intensity $|N_G|^2$ vs n, where $G = \frac{2\pi}{a} n$.

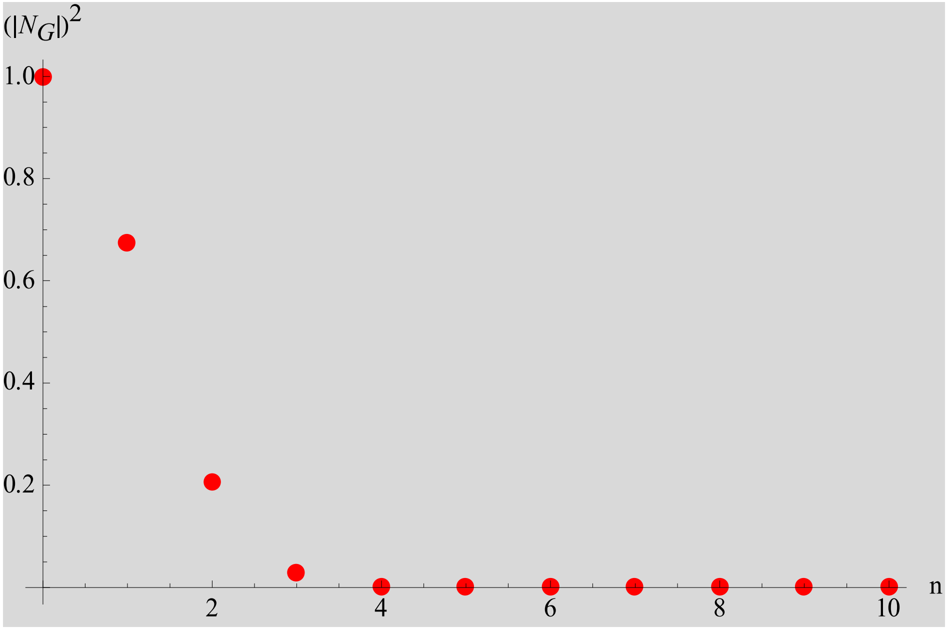


Fig. $a = 1$. $\sigma = 0.1$. $G = \frac{2\pi}{a} n$. The intensity $|N_G|^2$ vs n (= integer).

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