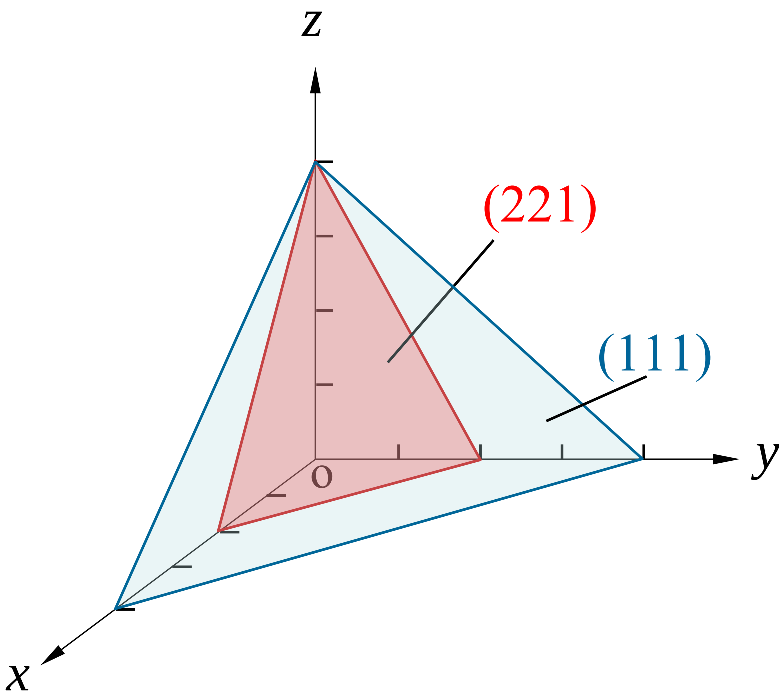
Reciprocal Lattice

The planes of lattices



Intercepts		Reciprocal	Miller indexes	
x	4	1/4	*h*	1
y	4	1/4	*k*	1
z	4	1/4	*l*	1
x	2	1/2	*h*	2
y	2	1/2	*k*	2
z	4	1/4	*l*	1

Reciprocal Lattice

What is it?   What is it for?   Why is it?

$$\begin{cases} \vec{b}_1 = \dfrac{\vec{a}_2 \times \vec{a}_3}{V} \\ \vec{b}_2 = \dfrac{\vec{a}_3 \times \vec{a}_1}{V} \\ \vec{b}_3 = \dfrac{\vec{a}_1 \times \vec{a}_2}{V} \end{cases} \quad (1)$$

$\vec{b}_j$ are the unit vectors in reciprocal space and not lying in the same plan.

$\vec{a}_i$ are the unit vectors in primitive space and not lying in the same plan.

V is the volume of unit cell and is written, for example, as $\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)$

or

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

- Periodicity of crystalline structure
- Periodicity of X-ray
- Definition of reciprocal lattice
- Mathematatic deduction

Periodicity of crystalline structure

Atoms in lattice consist of all points with position vectors $\vec{T}$ of the form.

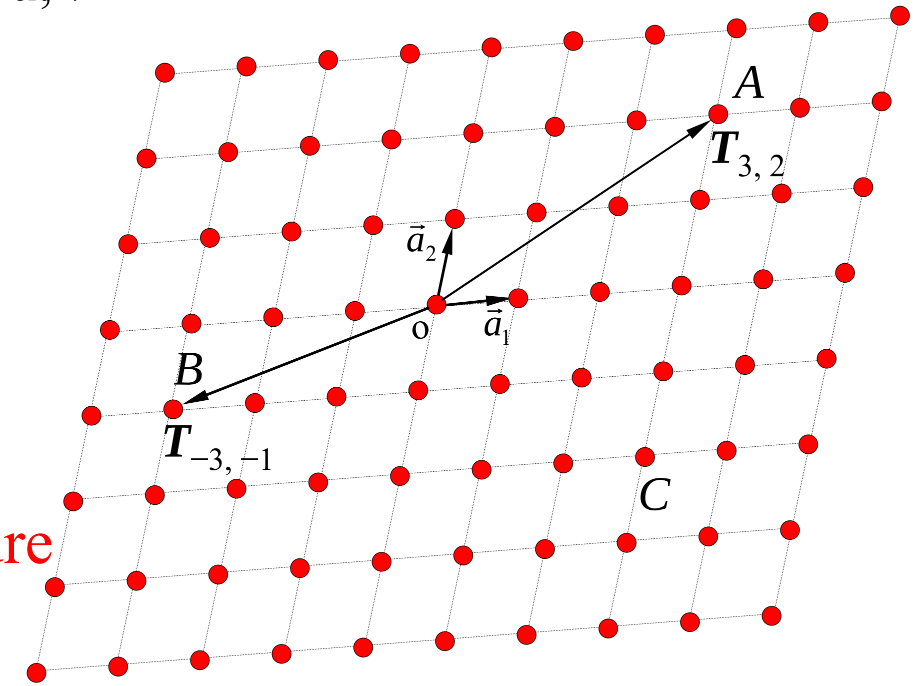
Translational symmetry

$$\vec{T} = u\vec{a}_1 + v\vec{a}_2 + w\vec{a}_3 \qquad (2)$$

$\vec{a}_1$, $\vec{a}_2$ and $\vec{a}_3$ are any three vectors in primitive space which are not all in the same plane. u, v and w range through all integral values.

$$\vec{T}_{3,2} = 3\vec{a}_1 + 2\vec{a}_2$$

$$\vec{T}_{-3,-1} = -3\vec{a}_1 - \vec{a}_2$$



The vectors of a unit cell of Bravais lattice, $\vec{a}_i$ (i = 1 , 2, 3), are given by

$$\vec{T}_0 = \vec{a}_1 + \vec{a}_2 + \vec{a}_3 \qquad (3)$$

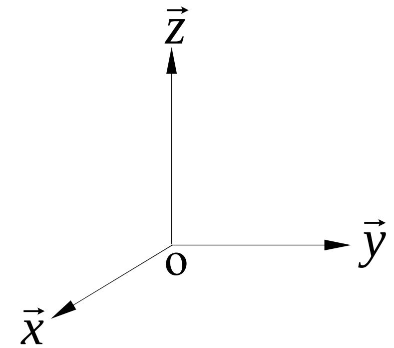
that determine the crystalline structure

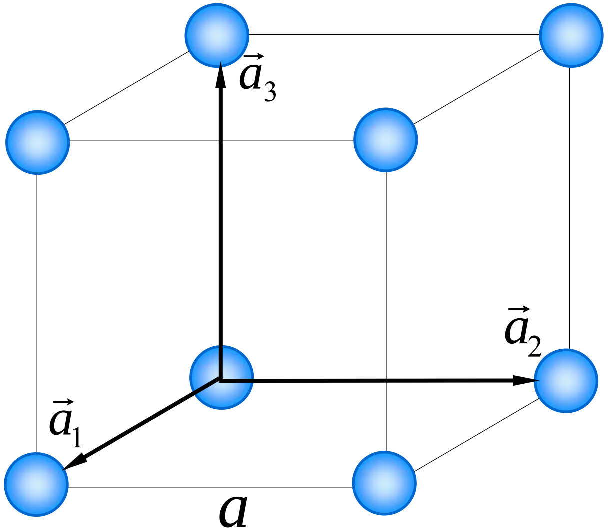
Vectors of a unit cell of Bravais lattice

(1) For a simple cubic (sc) lattice

$$\begin{cases} \vec{a}_1 = a\vec{x} \\ \vec{a}_2 = a\vec{y} \\ \vec{a}_3 = a\vec{z} \end{cases} \qquad (4)$$

Where $\vec{x}$, $\vec{y}$ and $\vec{z}$ are three orthogonal unit vectors in 'right hand' system.





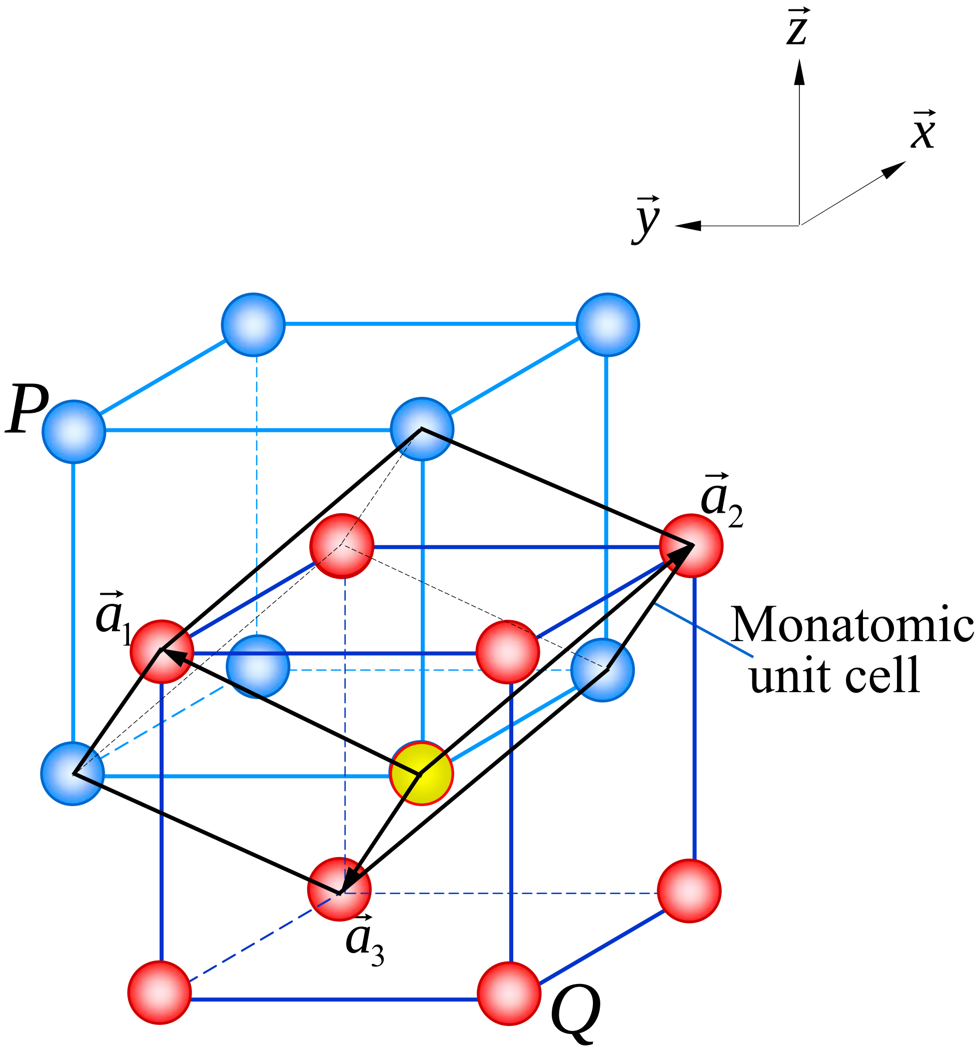
(2) For bcc lattice

A more symmetric system is

$$\left.\begin{aligned}\vec{a}_1 &= \frac{a}{2}(-\vec{x}+\vec{y}+\vec{z})\\ \vec{a}_2 &= \frac{a}{2}(\vec{x}-\vec{y}+\vec{z})\\ \vec{a}_3 &= \frac{a}{2}(\vec{x}+\vec{y}-\vec{z})\end{aligned}\right\} \quad (5)$$

$$P = 2\vec{a}_1 + \vec{a}_2 + \vec{a}_3$$

$$Q = -\vec{a}_1 - \vec{a}_2 - \vec{a}_3$$



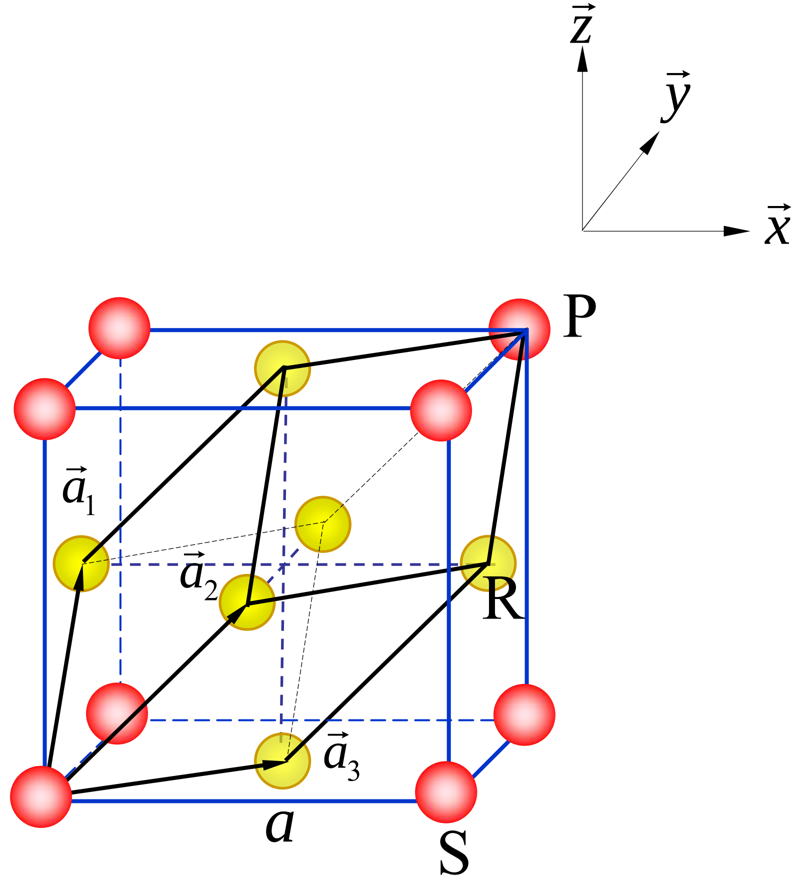
(3). For fcc lattice

$$\begin{cases} \vec{a}_1 = \dfrac{a}{2}(\vec{y}+\vec{z}) \\ \vec{a}_2 = \dfrac{a}{2}(\vec{x}+\vec{z}) \\ \vec{a}_3 = \dfrac{a}{2}(\vec{x}+\vec{y}) \end{cases} \qquad (6)$$

$$P = \vec{a}_1 + \vec{a}_2 + \vec{a}_3$$

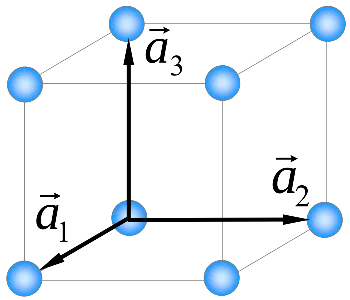
$$R = \vec{a}_2 + \vec{a}_3$$

$$S = -\vec{a}_1 + \vec{a}_2 + \vec{a}_3$$



$\vec{a}_1 \quad \vec{a}_2 \quad \vec{a}_3$

The unit vectors & the crystalline structure



Unit cell ← $\vec{T}_0 = \vec{a}_1 + \vec{a}_2 + \vec{a}_3$

The unit vectors determine crystalline structure !

Table 1. Unit vectors of the cell of cubic lattices

	$\vec{a}_1$	$\vec{a}_2$	$\vec{a}_3$
sc	$a\vec{x}$	$a\vec{y}$	$a\vec{z}$
bcc	$\frac{a}{2}(-\vec{x}+\vec{y}+\vec{z})$	$\frac{a}{2}(\vec{x}-\vec{y}+\vec{z})$	$\frac{a}{2}(\vec{x}+\vec{y}-\vec{z})$
fcc	$\frac{a}{2}(\vec{y}+\vec{z})$	$\frac{a}{2}(\vec{z}+\vec{x})$	$\frac{a}{2}(\vec{x}+\vec{y})$

where $\vec{x}, \vec{y}, \vec{z}$ are three orthogonal unit vectors in “right hand” system, and a is a lattice constant.

Periodicity of X-ray

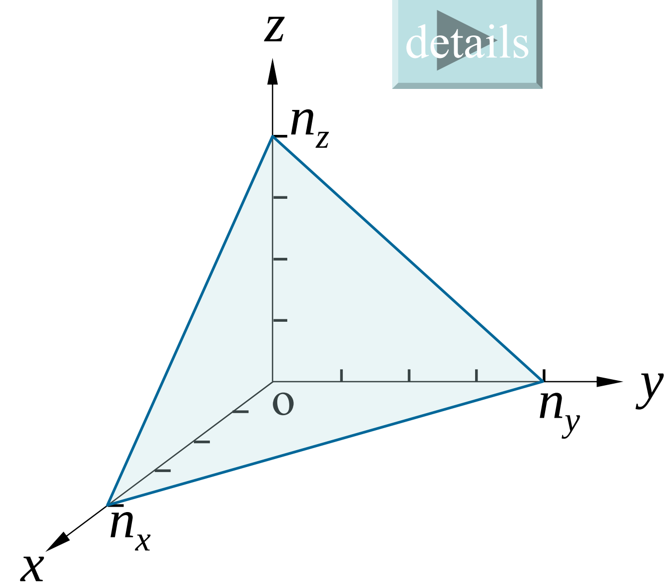
X-ray, in quantum mechanics, is given by a wave function

details

$$\psi = Ae^{i2\pi\vec{k}\cdot\vec{r}} \qquad (7)$$

$$\vec{k} = \frac{\vec{n}}{\lambda} \qquad \text{wave vector}$$

$$\vec{k} = h\vec{b}_1 + k\vec{b}_2 + l\vec{b}_3 \qquad (8)$$

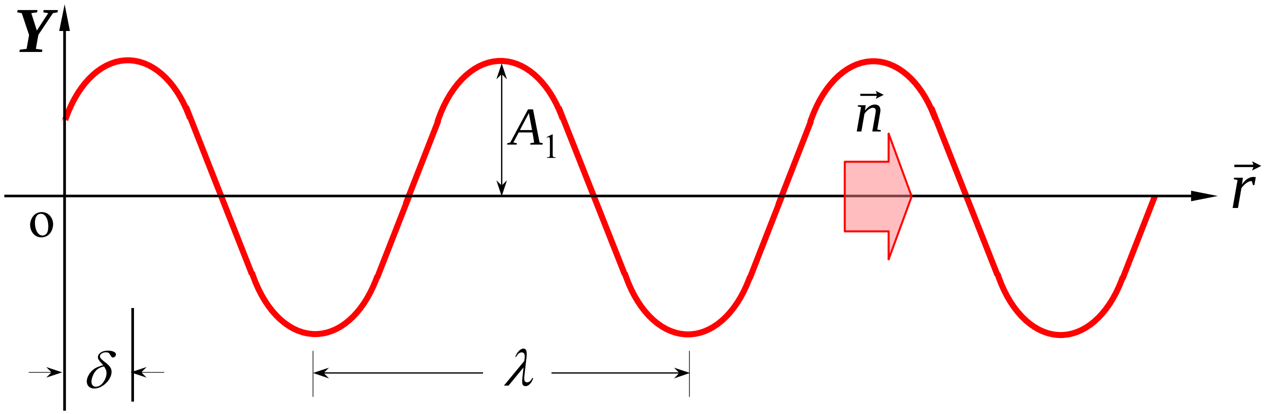


$\vec{b}_j$ are the unit vectors in reciprocal space and not lying in the same plane. *h*, *k* and *l* range through all integral values in reciprocal space.

$$h = 1/n_x$$
$$k = 1/n_y$$
$$l = 1/n_z$$

h, *k*, and *l* are Miller indexes of plane.

In classic theory, a harmonic wave is described in a **Wave Function** at a fixed time ($t = t_0$).



$$e^{i\theta} = \cos\theta + i\sin\theta$$

$$Y = A_1 \cdot \cos\left(2\pi \frac{\vec{n}\cdot\vec{r}}{\lambda} - \delta\right)$$

$$Y = Ae^{i2\pi\frac{\vec{n}\cdot\vec{r}}{\lambda}}$$

In quantum mechanics,
a **wave vector** is given as

$$\vec{k} = \frac{\vec{n}}{\lambda}$$

$$\vec{k} = 2\pi\frac{\vec{n}}{\lambda}$$

$$\psi = Ae^{i2\pi\vec{k}\cdot\vec{r}}$$

$$\psi = Ae^{i\vec{k}\cdot\vec{r}}$$

Definition of reciprocal lattice

Interaction between $\vec{T}$ and $\vec{k}$

$$\vec{T} = u\vec{a}_1 + v\vec{a}_2 + w\vec{a}_3 \qquad \text{Crystal}$$

$$\vec{k} = h\vec{b}_1 + k\vec{b}_2 + l\vec{b}_3 \qquad \text{X-Ray}$$

A wave vector $\vec{k}$ that yields plane wave with the periodicity of a given Bravais lattice $\vec{T}$ is known as **its reciprocal lattice, $\vec{K}$** details

$$\vec{K} = H\vec{b}_1 + K\vec{b}_2 + L\vec{b}_3$$

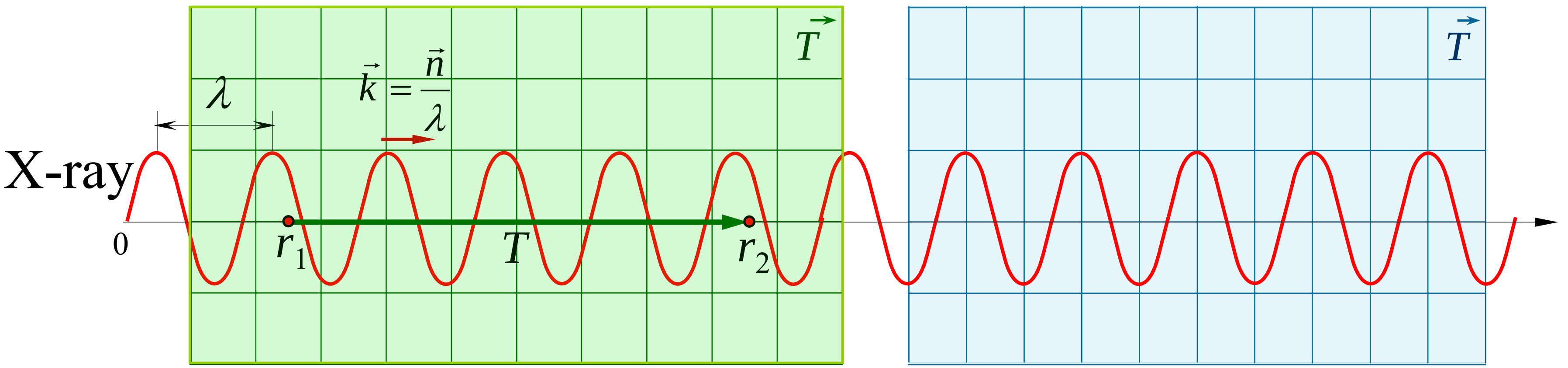
$\vec{K}$ with the same periodicity of given primitive lattice, $\vec{T}$

$$\vec{b}_j = f(\vec{a}_i)$$

X-ray and crystal

Interaction of $\vec{k}$ and $\vec{T}$, $\psi = Ae^{i2\pi\vec{k}\cdot\vec{r}} = \psi_r$

Amplitude
Probability



At point r_1, $\psi_{r_1} = Ae^{i2\pi\vec{k}\cdot\vec{r}_1}$ At point r_2, $\psi_{r_2} = Ae^{i2\pi\vec{k}\cdot\vec{r}_2}$

Let $r_2 - r_1 = T$, one finds that $\psi_{r_2} = Ae^{i2\pi\vec{k}\cdot(\vec{r}_1+\vec{T})}$

$\vec{k}$ with the same periodicity of primitive lattice, $\vec{T}$ $e^{i2\pi\vec{k}\cdot(\vec{r}+\vec{T})} = e^{i2\pi\vec{k}\cdot\vec{r}}$

$$\vec{k} \Rightarrow \vec{K} \quad e^{i2\pi\vec{K}\cdot(\vec{r}+\vec{T})} = e^{i2\pi\vec{K}\cdot\vec{r}}$$

$$\boxed{\vec{K} = H\vec{b}_1 + K\vec{b}_2 + L\vec{b}_3}$$

back

$\vec{K}$ with the same periodicity of given primitive lattice, $\vec{T}$

Mathematically

$$e^{i2\pi\vec{K}(\vec{r}+\vec{T})} = e^{i2\pi\vec{K}\cdot\vec{r}} \qquad (9)$$

$$e^{i2\pi\vec{K}\cdot\vec{T}} = 1 \qquad (10)$$

$$e^{i\theta} = \cos\theta + i\sin\theta$$

$$(-1)^{2\vec{K}\cdot\vec{T}} = 1$$

$$\vec{K}\cdot\vec{T} = \xi \quad (\xi = \text{integral}) \qquad (11)$$

$$\vec{K}\cdot\vec{T}=\xi$$

$$\vec{T}=u\vec{a}_1+v\vec{a}_2+w\vec{a}_3$$
$$\vec{K}=h\vec{b}_1+k\vec{b}_2+l\vec{b}_3$$

$$\vec{T}\cdot\vec{K}=(u\vec{a}_1+v\vec{a}_2+w\vec{a}_3)\cdot(hb_1+kb_2+lb_3)\ ?\ =uh+vk+wl$$

detail

$$=uh(\vec{a}_1\cdot\vec{b}_1)+vh(\vec{a}_2\cdot\vec{b}_1)+wh(\vec{a}_3\cdot\vec{b}_1)$$
$$+uk(\vec{a}_1\cdot\vec{b}_2)+vk(\vec{a}_2\cdot\vec{b}_2)+wk(\vec{a}_3\cdot\vec{b}_2)$$
$$+ul(\vec{a}_1\cdot\vec{b}_3)+vl(\vec{a}_2\cdot\vec{b}_3)+wl(\vec{a}_3\cdot\vec{b}_3)$$

$$\vec{a}_2\cdot\vec{b}_1=\vec{a}_3\cdot\vec{b}_1=0 \quad \vec{b}_1\perp(\vec{a}_2,\vec{a}_3) \quad \vec{b}_1=g_1(\vec{a}_2\times\vec{a}_3)$$
$$\vec{a}_1\cdot\vec{b}_2=\vec{a}_3\cdot\vec{b}_2=0 \quad \vec{b}_2\perp(\vec{a}_3,\vec{a}_1) \quad \vec{b}_2=g_2(\vec{a}_3\times\vec{a}_1)$$
$$\vec{a}_1\cdot\vec{b}_3=\vec{a}_2\cdot\vec{b}_3=0 \quad \vec{b}_3\perp(\vec{a}_1,\vec{a}_2) \quad \vec{b}_3=g_3(\vec{a}_1\times\vec{a}_2)$$

$$=\xi\begin{cases} n_i m_j=\text{integral} \\ \vec{a}_i\cdot\vec{b}_j=\begin{cases}1\ (i=j)\\ 0\ (i\neq j)\end{cases}\end{cases}$$

$$\vec{a}_1\cdot\vec{b}_1=\vec{a}_2\cdot\vec{b}_2=\vec{a}_3\cdot\vec{b}_3=1$$ ***Orthonormalization***

$$\vec{a}_1\cdot\vec{b}_1=1 \qquad \vec{a}_2\cdot\vec{b}_2=1 \qquad \vec{a}_3\cdot\vec{b}_3=1$$

$$(\vec{a}_2\times\vec{a}_3)\cdot\vec{a}_1\cdot\vec{b}_1=\vec{a}_2\times\vec{a}_3$$
$$V\cdot\vec{b}_1=\vec{a}_2\times\vec{a}_3$$

$$\vec{b}_1=\frac{\vec{a}_2\times\vec{a}_3}{V} \qquad \vec{b}_2=\frac{\vec{a}_3\times\vec{a}_1}{V} \qquad \vec{b}_3=\frac{\vec{a}_1\times\vec{a}_2}{V}$$

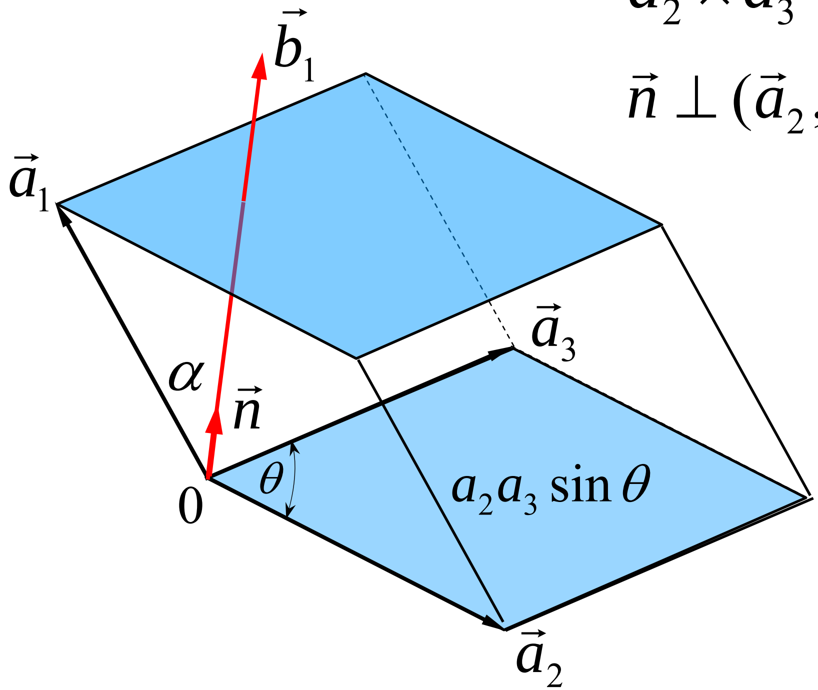
$$\vec{a}_i\cdot\vec{b}_j=\delta_{ij} \qquad \begin{cases}\delta_{ij}=0,\ i\neq j\\ \delta_{ij}=1,\ i=j\end{cases}$$

Kronecker delta symbol

$\vec{b}_1 = g_1(\vec{a}_2 \times \vec{a}_3)$ $\vec{b}_1 // \vec{n} \perp (\vec{a}_2, \vec{a}_3)$

$\vec{a}_2 \times \vec{a}_3 = (a_2 a_3 \sin\theta)\vec{n}$

$\vec{n} \perp (\vec{a}_2, \vec{a}_3)$



$$V = \vec{a}_1(\vec{a}_2 \times \vec{a}_3) = a_1(a_2 a_3 \sin\theta)\cos\alpha$$

back

$$\begin{cases} \vec{b}_1 = \dfrac{\vec{a}_2 \times \vec{a}_3}{V} \\ \vec{b}_2 = \dfrac{\vec{a}_3 \times \vec{a}_1}{V} \\ \vec{b}_3 = \dfrac{\vec{a}_1 \times \vec{a}_2}{V} \end{cases} \qquad (1)$$

$\vec{b}_j$ are the unit vectors in reciprocal space and not in the same plan.

$\vec{a}_i$ are the unit vectors in primitive space and not in the same plan.

V is the volume of UC which can be written, for example, as $\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)$

$$\vec{k} = \frac{\vec{n}}{\lambda}$$

(hkl)

$$\vec{k} \propto \frac{1}{\lambda}$$

$$\vec{k} = 2\pi \frac{\vec{n}}{\lambda}$$

$$b_j \propto \frac{1}{a_i}$$

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

Summary for reciprocal lattices

1) What is it ? 传道

2) What is it for ? 授业

3) Why is it ? 解惑

"What is it ?" The definition of RL

$$\begin{cases} \vec{b}_1 = \dfrac{\vec{a}_2 \times \vec{a}_3}{V} \\ \vec{b}_2 = \dfrac{\vec{a}_3 \times \vec{a}_1}{V} \\ \vec{b}_3 = \dfrac{\vec{a}_1 \times \vec{a}_2}{V} \end{cases} \quad (1)$$

$\vec{b}_j$ are the unit vectors in reciprocal space and not lying in the same plan.

$\vec{a}_i$ are the unit vectors in primitive space and not lying in the same plan.

V is the volume of unit cell and is written, for example, as $\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)$

What is it for ?

Characterization of reciprocal lattice

1) Plane (*kkl*) in primitive space is perpendicular to the reciprocal vector

$$\vec{K} = h\vec{b}_1 + k\vec{b}_2 + l\vec{b}_3$$

2) The spacing of the plane (*kkl*) is given to $d_{hkl} = \frac{1}{|\vec{K}|}$

3) Relations between primitive lattice and reciprocal lattice

$$\mathrm{FCC_R} \leftrightarrows \mathrm{BCC_P} \qquad \mathrm{BCC_R} \leftrightarrows \mathrm{FCC_P}$$

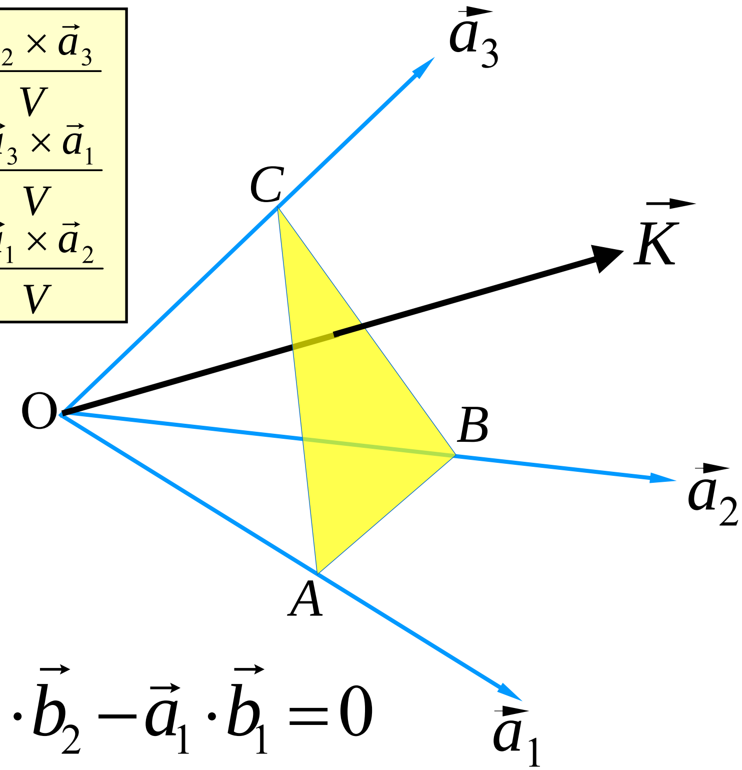
【Example 1】

Plane (*kkl*) is **perpendicular** to the reciprocal vector $\vec{K} = h\vec{b}_1 + k\vec{b}_2 + l\vec{b}_3$

$$\vec{K} \perp \vec{AB} \;\Rightarrow\; \vec{K}\cdot\vec{AB} = 0$$

$$\vec{K} \perp \vec{AC} \;\Rightarrow\; \vec{K}\cdot\vec{AC} = 0$$

$$\vec{b}_1 = \frac{\vec{a}_2 \times \vec{a}_3}{V} \qquad \vec{b}_2 = \frac{\vec{a}_3 \times \vec{a}_1}{V} \qquad \vec{b}_3 = \frac{\vec{a}_1 \times \vec{a}_2}{V}$$



$$\vec{OA} = \frac{\vec{a}_1}{h} \qquad \vec{OB} = \frac{\vec{a}_2}{k} \qquad \vec{OC} = \frac{\vec{a}_3}{l}$$

$$\vec{AB} = \vec{OB} - \vec{OA} = \frac{\vec{a}_2}{k} - \frac{\vec{a}_1}{h}$$

$$\vec{K}\cdot\vec{AB} = (h\vec{b}_1 + k\vec{b}_2 + l\vec{b}_3)\cdot\left(\frac{\vec{a}_2}{k} - \frac{\vec{a}_1}{h}\right) = \vec{a}_2\cdot\vec{b}_2 - \vec{a}_1\cdot\vec{b}_1 = 0$$

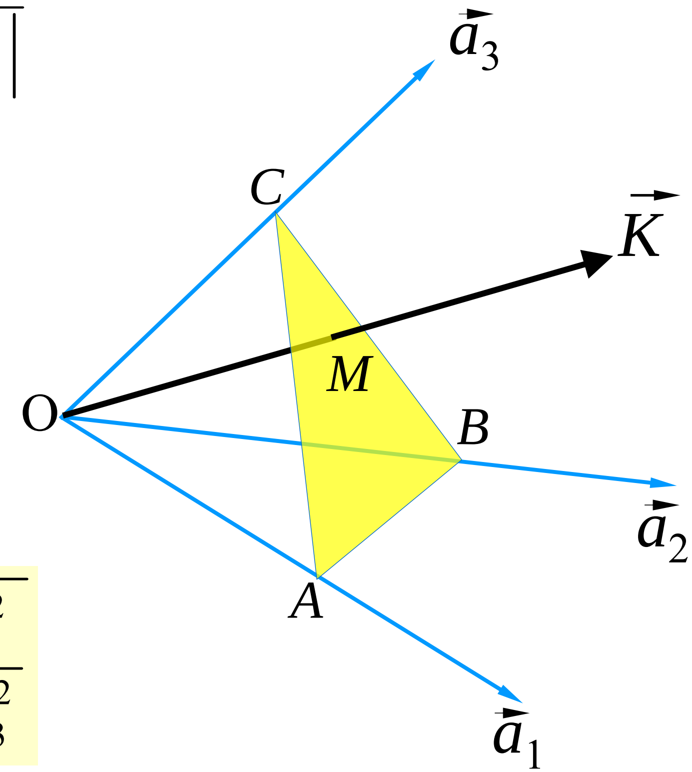
$$\vec{AC} = \vec{OC} - \vec{OA} = \frac{\vec{a}_3}{l} - \frac{\vec{a}_1}{h}$$

$$\vec{K}\cdot\vec{AC} = (h\vec{b}_1 + k\vec{b}_2 + l\vec{b}_3)\cdot\left(\frac{\vec{a}_3}{l} - \frac{\vec{a}_1}{h}\right) = \vec{a}_3\cdot\vec{b}_3 - \vec{a}_1\cdot\vec{b}_1 = 0$$

back

【Example 2】 The spacing of the plane (kkl) $d_{hkl} = 1/|\vec{K}|$

$$d_{hkl} = \overline{OM} = \overrightarrow{OA} \cdot \frac{\vec{K}}{|\vec{K}|} = \frac{\vec{a}_1}{h} \cdot \frac{(h\vec{b}_1 + k\vec{b}_2 + l\vec{b}_3)}{|\vec{K}|} = \frac{1}{|\vec{K}|}$$



$$\vec{K} = h\vec{b}_1 + k\vec{b}_2 + l\vec{b}_3$$

$$|\vec{K}| = \sqrt{(h\vec{b}_1)^2 + (k\vec{b}_2)^2 + (l\vec{b}_3)^2}$$

$$\begin{cases} \vec{b}_1 = \dfrac{\vec{a}_2 \times \vec{a}_3}{V} = \dfrac{\vec{n}_1}{a_1} \\ \vec{b}_2 = \dfrac{\vec{a}_3 \times \vec{a}_1}{V} = \dfrac{\vec{n}_2}{a_2} \\ \vec{b}_3 = \dfrac{\vec{a}_1 \times \vec{a}_2}{V} = \dfrac{\vec{n}_3}{a_3} \end{cases}$$

$$|\vec{K}| = \sqrt{\frac{h^2}{a_1^2} + \frac{k^2}{a_2^2} + \frac{l^2}{a_3^2}}$$

$$d_{hkl} = \frac{1}{|\vec{K}|}$$

$$\frac{1}{d_{hkl}^2} = \frac{h^2}{a_1^{\,2}} + \frac{k^2}{a_2^{\,2}} + \frac{l^2}{a_3^{\,2}}$$

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【Example 3】

Simple cubic (sc) lattice

Reciprocal lattice

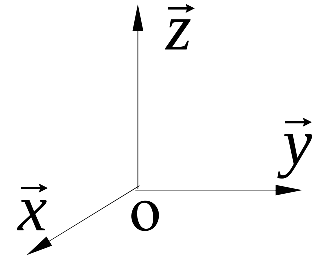
$$\vec{b}_1 = \frac{\vec{a}_2 \times \vec{a}_3}{V} \qquad \vec{b}_2 = \frac{\vec{a}_3 \times \vec{a}_1}{V} \qquad \vec{b}_3 = \frac{\vec{a}_1 \times \vec{a}_2}{V}$$

$$\vec{a}_1 = a\vec{x} \qquad \vec{a}_2 = a\vec{y} \qquad \vec{a}_3 = a\vec{z} \qquad (3)$$

$$\vec{b}_1 = \frac{\vec{a}_2 \times \vec{a}_3}{V} = \frac{a\vec{y} \times a\vec{z}}{a^3} = \frac{1}{a}\vec{y} \times \vec{z} = \frac{1}{a}\vec{x}$$

Similarly

$$\vec{b}_2 = \frac{1}{a}\vec{y} \qquad \vec{b}_3 = \frac{1}{a}\vec{z} \qquad (13)$$



$\vec{b}_i$ construct another sc Bravais lattice

For the sc lattice, both primitive and reciprocal lattices have the same structure. (Q: what is their difference)

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【Example 4】

Face-centered cubic (fcc) lattice

Reciprocal lattice

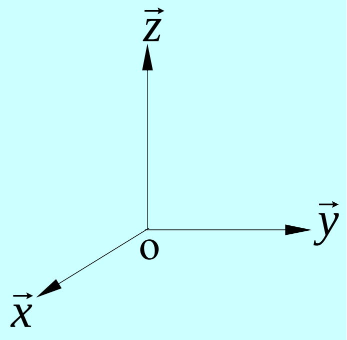
$$\vec{b}_1 = \frac{\vec{a}_2 \times \vec{a}_3}{V} \qquad \vec{b}_2 = \frac{\vec{a}_3 \times \vec{a}_1}{V} \qquad \vec{b}_3 = \frac{\vec{a}_1 \times \vec{a}_2}{V}$$

$$\vec{a}_1 = \frac{a}{2}(\vec{y}+\vec{z}) \quad \vec{a}_2 = \frac{a}{2}(\vec{z}+\vec{x}) \quad \vec{a}_3 = \frac{a}{2}(\vec{x}+\vec{y}) \qquad \textbf{(6)}$$

$$\vec{b}_1 = \frac{\vec{a}_2 \times \vec{a}_3}{V} = \frac{\frac{a}{2}(\vec{z}+\vec{x}) \times \frac{a}{2}(\vec{x}+\vec{y})}{a^3}$$

$$= \frac{1}{4a}(\vec{z}+\vec{x})\times(\vec{x}+\vec{y}) = \frac{1}{4a}(\vec{z}\times\vec{x}+\vec{z}\times\vec{y}+\vec{x}\times\vec{x}+\vec{x}\times\vec{y})$$

$$= \frac{1}{4a}(\vec{y}-\vec{x}+\vec{z})$$



Therefore, one can find that

$$\begin{cases} \vec{b}_1 = \frac{1}{4a}(-\vec{x}+\vec{y}+\vec{z}) \\ \vec{b}_2 = \frac{1}{4a}(\vec{x}-\vec{y}+\vec{z}) \\ \vec{b}_3 = \frac{1}{4a}(\vec{x}+\vec{y}-\vec{z}) \end{cases} \qquad (14)$$

Body-centered cubic **(5)**

Table 2. Relation of primitive and reciprocal lattices

Primitive lattice	Reciprocal lattice
Simple cubic	Simple cubic
Face-centered cubic	Body-centered cubic
Body-centered cubic	Face-centered cubic

"Why is it?" *K* + *T* → RL

crystal & X-ray

$$\vec{T} = u\vec{a}_1 + v\vec{a}_2 + w\vec{a}_3$$

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

⇨

Reciprocal Lattice

$\vec{k}$ has same periodicity with $\vec{T}$

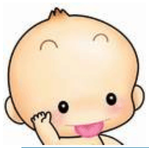
⇨

$$\cdot\vec{T} = \xi$$

⇨

$$\begin{cases} \vec{b}_1 = \dfrac{\vec{a}_2 \times \vec{a}_3}{V} \\ \vec{b}_2 = \dfrac{\vec{a}_3 \times \vec{a}_1}{V} \\ \vec{b}_3 = \dfrac{\vec{a}_1 \times \vec{a}_2}{V} \end{cases}$$

Home works



PROBLEMS

- Prove that $\vec{a}_1 \cdot \vec{b}_1 = 1$ and $\vec{a}_2 \cdot \vec{b}_1 = 0$
- Prove that $\vec{a}_1 // \vec{b}_1 // \vec{x}$ in cubic lattices.

$$\vec{a}_2 // \vec{b}_2 // \vec{y}$$
$$\vec{a}_3 // \vec{b}_3 // \vec{z}$$

- Prove that the reciprocal lattice of FCC is a BCC structure.