

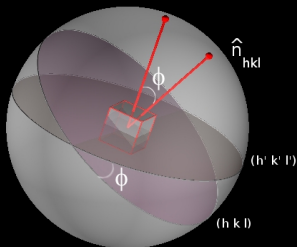
Reciprocal space

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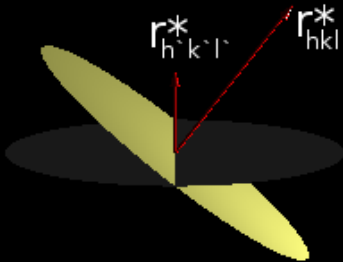
IUCr International School on Crystallography, La Plata,
2014.

Definition



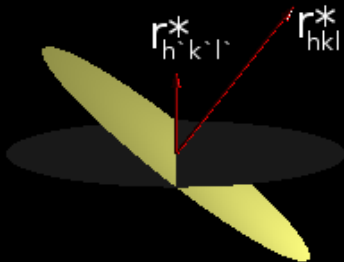
While constructing the stereographic projection we saw that the angle between planes could be also measured as the angles between the corresponding normal.

Definition



We can add metric information to the normals by associating the norm of the vector somehow to the interplanar distance.

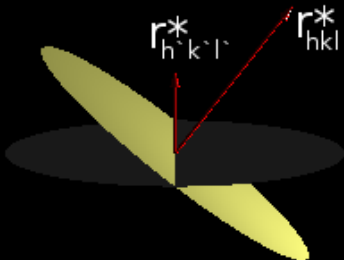
Definition



We can add metric information to the normals by associating the norm of the vector somehow to the interplanar distance.

The reciprocal vector r_{hkl}^* is defined as a vector normal to plane (hkl) with length $1/d_{hkl}$

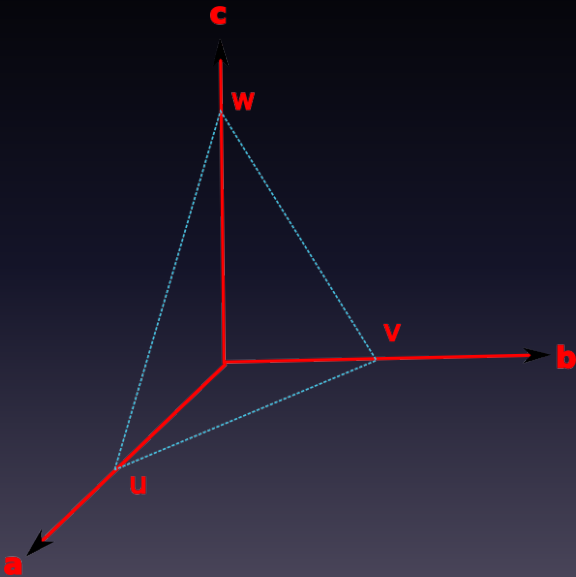
Definition



$$\vec{r}_{hkl}^* \parallel n_{hkl}$$

$$|\vec{r}_{hkl}^*| = \frac{1}{d_{hkl}}$$

Equation of a plane



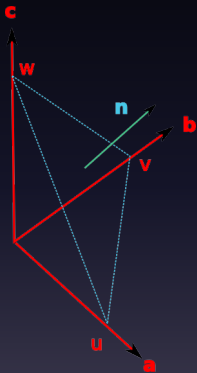
$$(u, 0, 0) \quad (0, v, 0) \quad (0, 0, w)$$

$$\vec{u} = u\vec{a}$$

$$\vec{v} = v\vec{b}$$

$$\vec{w} = w\vec{c}$$

Equation of a plane

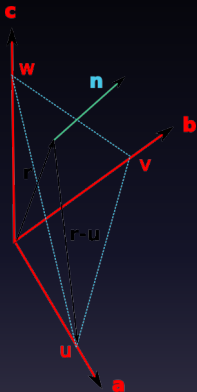


$$\vec{n} = (\vec{u} - \vec{v}) \times (\vec{v} - \vec{w})$$

$$\vec{n} = (\vec{v} \times \vec{w}) + (\vec{w} \times \vec{u}) + (\vec{u} \times \vec{v})$$

$$\vec{n} = vw(\vec{b} \times \vec{c}) + uw(\vec{c} \times \vec{a}) + uv(\vec{a} \times \vec{b})$$

Equation of a plane



$$\vec{n} \cdot (\vec{r} - \vec{u}) = 0$$

$$\vec{n} \cdot \vec{r} = \vec{n} \cdot \vec{u}$$

$$\vec{n} = vw(\vec{b} \times \vec{c}) + uw(\vec{c} \times \vec{a}) + uv(\vec{a} \times \vec{b})$$
$$\vec{r} = x\vec{a} + y\vec{b} + z\vec{c}$$

$$vw x (\vec{b} \times \vec{c}) \cdot \vec{a} + uw y (\vec{c} \times \vec{a}) \cdot \vec{b} + uv z (\vec{a} \times \vec{b}) \cdot \vec{c} =$$
$$uvw (\vec{b} \times \vec{c}) \cdot \vec{a}$$

Equation of a plane

$$vwx(\vec{b} \times \vec{c}) \cdot \vec{a} + uwy(\vec{c} \times \vec{a}) \cdot \vec{b} + uvz(\vec{a} \times \vec{b}) \cdot \vec{c} =$$
$$uvw(\vec{b} \times \vec{c}) \cdot \vec{a}$$

Equation of a plane

$$vwx(\vec{b} \times \vec{c}) \cdot \vec{a} + uwy(\vec{c} \times \vec{a}) \cdot \vec{b} + uvz(\vec{a} \times \vec{b}) \cdot \vec{c} =$$
$$uvw(\vec{b} \times \vec{c}) \cdot \vec{a}$$

$$\frac{x}{u} \left[\frac{\vec{b} \times \vec{c}}{\vec{a} \cdot (\vec{b} \times \vec{c})} \right] \cdot \vec{a} + \frac{y}{v} \left[\frac{\vec{c} \times \vec{a}}{\vec{a} \cdot (\vec{b} \times \vec{c})} \right] \cdot \vec{b} + \frac{z}{w} \left[\frac{\vec{a} \times \vec{b}}{\vec{a} \cdot (\vec{b} \times \vec{c})} \right] \cdot \vec{c} = 1$$

Equation of a plane

$$vwx(\vec{b} \times \vec{c}) \cdot \vec{a} + uwy(\vec{c} \times \vec{a}) \cdot \vec{b} + uvz(\vec{a} \times \vec{b}) \cdot \vec{c} =$$
$$uvw(\vec{b} \times \vec{c}) \cdot \vec{a}$$

$$\frac{x}{u} \left[\frac{\vec{b} \times \vec{c}}{\vec{a} \cdot (\vec{b} \times \vec{c})} \right] \cdot \vec{a} + \frac{y}{v} \left[\frac{\vec{c} \times \vec{a}}{\vec{a} \cdot (\vec{b} \times \vec{c})} \right] \cdot \vec{b} + \frac{z}{w} \left[\frac{\vec{a} \times \vec{b}}{\vec{a} \cdot (\vec{b} \times \vec{c})} \right] \cdot \vec{c} = 1$$

$$\vec{a}^* = \frac{\vec{b} \times \vec{c}}{\vec{a} \cdot (\vec{b} \times \vec{c})}$$

$$\vec{b}^* = \frac{\vec{c} \times \vec{a}}{\vec{a} \cdot (\vec{b} \times \vec{c})}$$

$$\vec{c}^* = \frac{\vec{a} \times \vec{b}}{\vec{a} \cdot (\vec{b} \times \vec{c})}$$

Equation of a plane

$$\vec{a}^* = \frac{\vec{b} \times \vec{c}}{\vec{a} \cdot (\vec{b} \times \vec{c})}$$

$$\vec{b}^* = \frac{\vec{c} \times \vec{a}}{\vec{a} \cdot (\vec{b} \times \vec{c})}$$

$$\vec{c}^* = \frac{\vec{a} \times \vec{b}}{\vec{a} \cdot (\vec{b} \times \vec{c})}$$

$$\vec{a} \cdot \vec{a}^* = 1$$

$$\vec{b} \cdot \vec{a}^* = 0$$

$$\vec{c} \cdot \vec{a}^* = 0$$

$$\vec{a} \cdot \vec{b}^* = 0$$

$$\vec{b} \cdot \vec{b}^* = 1$$

$$\vec{c} \cdot \vec{b}^* = 0$$

$$\vec{a} \cdot \vec{c}^* = 0$$

$$\vec{b} \cdot \vec{c}^* = 0$$

$$\vec{c} \cdot \vec{c}^* = 1$$

Equation of a plane

$$\frac{x}{u} \left[\frac{\vec{b} \times \vec{c}}{\vec{a} \cdot (\vec{b} \times \vec{c})} \right] \cdot \vec{a} + \frac{y}{v} \left[\frac{\vec{c} \times \vec{a}}{\vec{a} \cdot (\vec{b} \times \vec{c})} \right] \cdot \vec{b} + \frac{z}{w} \left[\frac{\vec{a} \times \vec{b}}{\vec{a} \cdot (\vec{b} \times \vec{c})} \right] \cdot \vec{c} = 1$$

Equation of a plane

$$\frac{x}{u} \left[\frac{\vec{b} \times \vec{c}}{\vec{a} \cdot (\vec{b} \times \vec{c})} \right] \cdot \vec{a} + \frac{y}{v} \left[\frac{\vec{c} \times \vec{a}}{\vec{a} \cdot (\vec{b} \times \vec{c})} \right] \cdot \vec{b} + \frac{z}{w} \left[\frac{\vec{a} \times \vec{b}}{\vec{a} \cdot (\vec{b} \times \vec{c})} \right] \cdot \vec{c} = 1$$

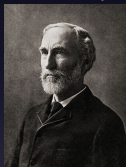
$$(x\vec{a}) \cdot (h\vec{a}^*) + (y\vec{b}) \cdot (k\vec{b}^*) + (z\vec{c}) \cdot (l\vec{c}^*) = 1$$

Equation of the plane

$$hx + ky + lz = 1$$

Some history

Gibbs (1839-1903)



Gibbs introduced the reciprocal base $\{\vec{a}_j^*\}$ from the condition $\vec{a}_i \cdot \vec{a}_j^* = K \delta_{ij}$

Reciprocal vector

$$(x\vec{a}) \cdot (h\vec{a}^*) + (y\vec{b}) \cdot (k\vec{b}^*) + (z\vec{c}) \cdot (l\vec{c}^*) = 1$$

$$hx + ky + lz = 1$$

can be written as

$$r_{xyz} \cdot r_{hkl}^* = 1$$

where

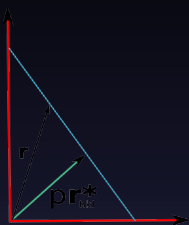
$$r_{hkl}^* = h\vec{a}^* + k\vec{b}^* + l\vec{c}^*$$

if

$$r_{hkl}^* \parallel \hat{n}_{hkl}$$

$$|r_{hkl}^*| = \frac{1}{d_{hkl}}$$

Reciprocal vector



Now by construction

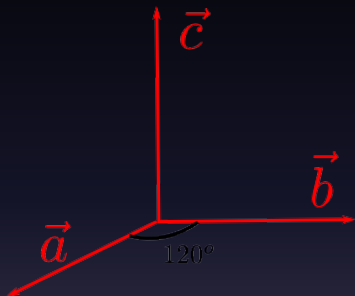
$$r_{hkl}^* \cdot (\vec{r} - pr_{hkl}^*) = 0$$

$$p|r_{hkl}^*|^2 = \vec{r} \cdot r_{hkl}^* = 1$$

$$p = \frac{1}{|r_{hkl}^*|^2}$$

$$p|r_{hkl}^*| = d_{hkl} \Rightarrow |r_{hkl}^*| = \frac{1}{d_{hkl}}$$

Reciprocal vector



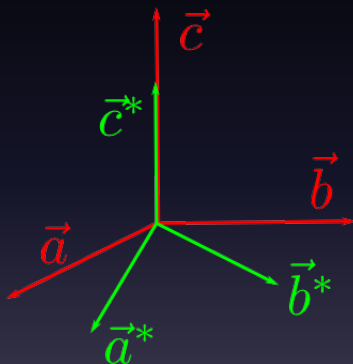
$$\begin{aligned}\vec{a} &= \vec{b} \neq \vec{c} \\ \alpha &= \beta = \frac{\pi}{2} \\ \gamma &= \frac{2\pi}{3}\end{aligned}$$

Hexagonal crystal basis

Find the reciprocal basis. Write the reciprocal metric tensor G^* .

Calculate $G \cdot G^*$.

Reciprocal vector



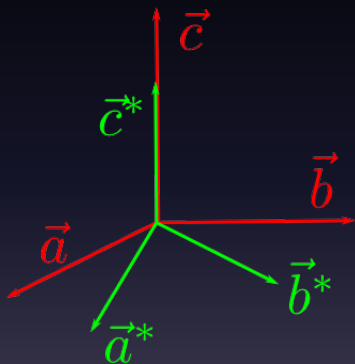
$$a^* = b^* = \frac{2}{\sqrt{3}} \frac{1}{a}$$

$$c^* = \frac{1}{c}$$

$$\alpha^* = \beta^* = \frac{\pi}{2}$$

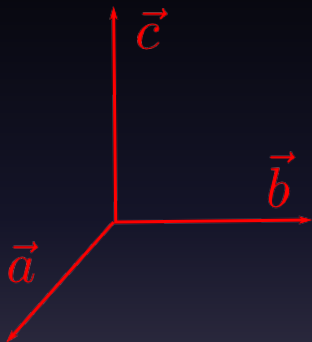
$$\gamma^* = \frac{\pi}{3}$$

Reciprocal vector



$$G^* = \begin{pmatrix} \frac{4}{3} \frac{1}{a^2} & \frac{2}{3} \frac{1}{a^2} & 0 \\ \frac{2}{3} \frac{1}{a^2} & \frac{4}{3} \frac{1}{a^2} & 0 \\ 0 & 0 & 1/c^2 \end{pmatrix}$$

Reciprocal vector



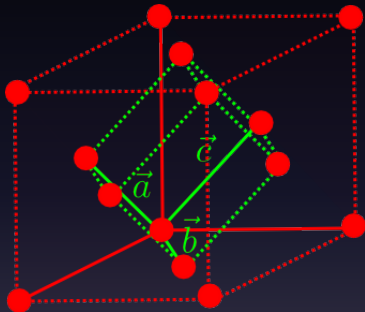
$$\vec{a} = \vec{b} \neq \vec{c}$$
$$\alpha = \beta = \gamma = \frac{\pi}{2}$$

Tetragonal crystal basis

Find the reciprocal basis. Write the reciprocal metric tensor G^* .

Calculate $G \cdot G^*$.

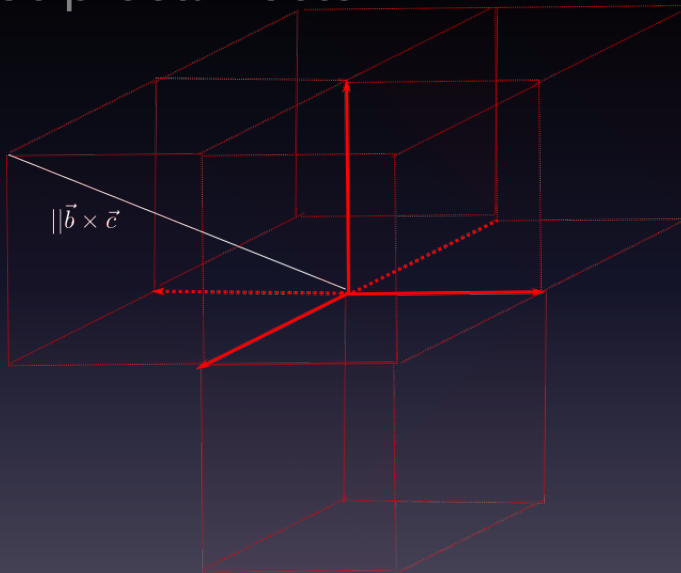
Reciprocal vector



FCC crystal basis

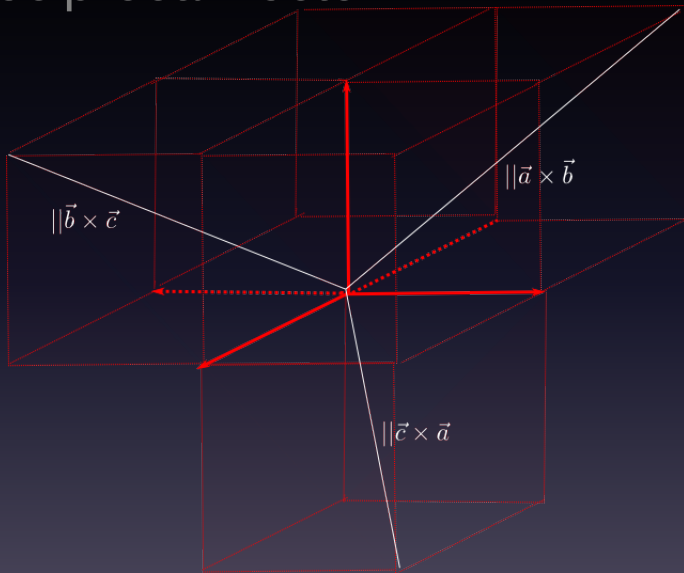
Find the reciprocal basis.

Reciprocal vector



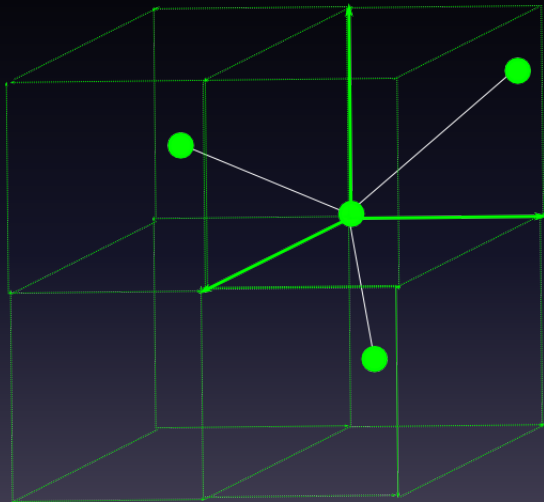
FCC crystal basis

Reciprocal vector



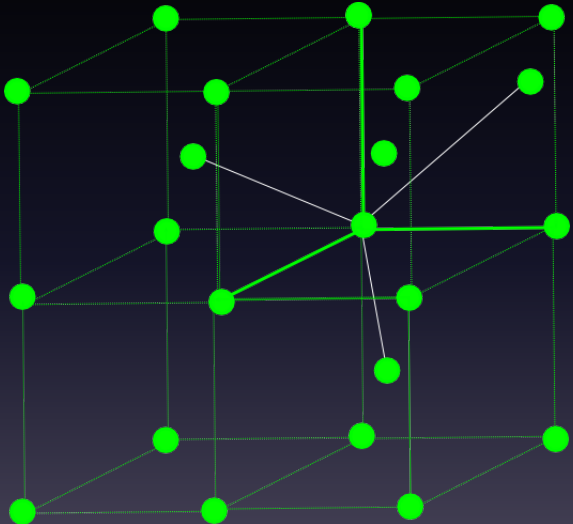
FCC crystal basis

Reciprocal vector



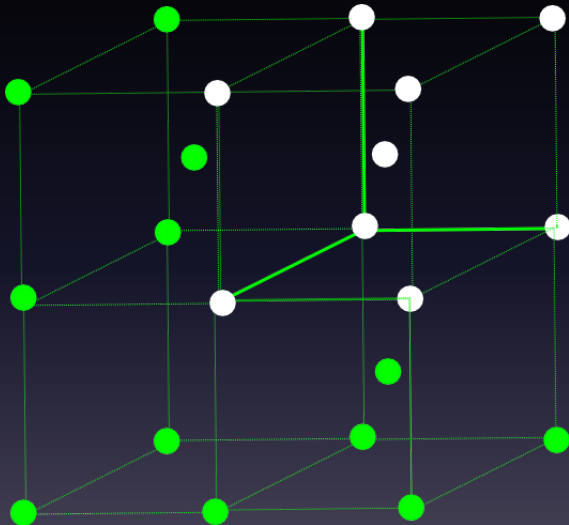
FCC crystal basis

Reciprocal vector



FCC crystal basis

Reciprocal vector

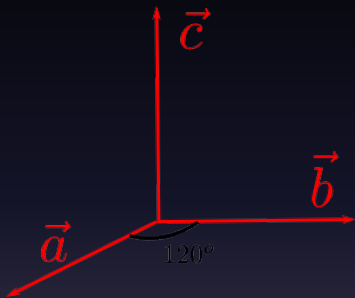


FCC crystal basis BCC reciprocal basis

Reciprocal vector

$$G \cdot G^* = I$$

Reciprocal vector

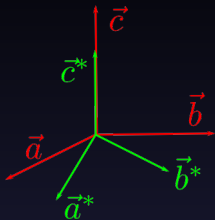


$$\begin{aligned}\vec{a} &= \vec{b} \neq \vec{c} \\ \alpha &= \beta = \frac{\pi}{2} \\ \gamma &= \frac{2\pi}{3}\end{aligned}$$

Hexagonal crystal basis

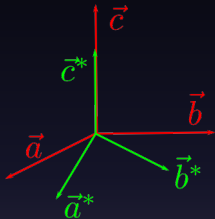
From the reciprocal metric tensor, find the interplara distance of the plane (hkl) .

Reciprocal vector



$$\frac{1}{d_{hkl}^2} = \vec{r}^* \cdot \vec{r}^* = (h \ k \ l) \begin{pmatrix} \frac{4}{3} \frac{1}{a^2} & \frac{2}{3} \frac{1}{a^2} & 0 \\ \frac{2}{3} \frac{1}{a^2} & \frac{4}{3} \frac{1}{a^2} & 0 \\ 0 & 0 & 1/c^2 \end{pmatrix} \begin{pmatrix} h \\ k \\ l \end{pmatrix}$$

Reciprocal vector



$$\frac{1}{d_{hkl}^2} = \vec{r}^* \cdot \vec{r}^* = \frac{4}{3} \frac{h^2 + hk + k^2}{a^2} + \frac{l^2}{c^2}$$

Coordinates transformations

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = F \cdot \begin{pmatrix} x \\ y \\ z \end{pmatrix}$$

$$\vec{r} = (\vec{a} \vec{b} \vec{c}) \cdot \begin{pmatrix} x \\ y \\ z \end{pmatrix} = (\vec{a}' \vec{b}' \vec{c}') \cdot \begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = (\vec{a}' \vec{b}' \vec{c}') \cdot F \cdot \begin{pmatrix} x \\ y \\ z \end{pmatrix}$$

from where

Basis transformation

$$(\vec{a}' \vec{b}' \vec{c}') = (\vec{a} \vec{b} \vec{c}) \cdot F^{-1}$$

Metric tensor transformations

$$\vec{r} \cdot \vec{r} = (x \ y \ z) \cdot G \cdot \begin{pmatrix} x \\ y \\ z \end{pmatrix} = (x' \ y' \ z') \cdot G' \cdot \begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = \\ (x \ y \ z) \cdot F^T \cdot G' \cdot F \cdot \begin{pmatrix} x \\ y \\ z \end{pmatrix}$$

from where calling $M = (F^T)^{-1}$

Metric tensor transformation

$$G' = M \cdot G \cdot M^T$$

Metric tensor transformations

$$\begin{pmatrix} \vec{a}^* \\ \vec{b}^* \\ \vec{c}^* \end{pmatrix} = G^* \cdot \begin{pmatrix} \vec{a} \\ \vec{b} \\ \vec{c} \end{pmatrix}$$

$$\begin{pmatrix} \vec{a} \\ \vec{b} \\ \vec{c} \end{pmatrix} = G \cdot \begin{pmatrix} \vec{a}^* \\ \vec{b}^* \\ \vec{c}^* \end{pmatrix}$$

Transformation in reciprocal space

$$\begin{aligned} \vec{r}^* &= (hkl) \cdot \begin{pmatrix} \vec{a}^* \\ \vec{b}^* \\ \vec{c}^* \end{pmatrix} = (h'k'l') \cdot \begin{pmatrix} \vec{a}^{*'} \\ \vec{b}^{*'} \\ \vec{c}^{*'} \end{pmatrix} = \\ (hkl) \cdot G^{-1} \cdot \begin{pmatrix} \vec{a} \\ \vec{b} \\ \vec{c} \end{pmatrix} &= (hkl) \cdot G^{-1} \cdot F^T \begin{pmatrix} \vec{a}' \\ \vec{b}' \\ \vec{c}' \end{pmatrix} = \\ &= (hkl) \cdot G^{-1} \cdot F^T \cdot G' \begin{pmatrix} \vec{a}^{*'} \\ \vec{b}^{*'} \\ \vec{c}^{*'} \end{pmatrix} \end{aligned}$$

Transformation in reciprocal space

$$\vec{r}^* = (h \ k \ l) \cdot \begin{pmatrix} \vec{a}^* \\ \vec{b}^* \\ \vec{c}^* \end{pmatrix} = (h \ k \ l) \cdot G^{-1} \cdot F^T \cdot G' \begin{pmatrix} \vec{a}^{*'} \\ \vec{b}^{*'} \\ \vec{c}^{*'} \end{pmatrix}$$

Now

$$G' = M \cdot G \cdot M^T = (F^T)^{-1} \cdot G \cdot F^{-1}$$

and finally

Reciprocal coordinates

$$(h' \ k' \ l') = (h \ k \ l) \cdot M^T = (h \ k \ l) \cdot F^{-1}$$

Point symmetry transformation in reciprocal space

Let R be a point symmetry operation acting over the coordinates of the atoms, then according to the transformation rules already derived

$$(h^e k^e l^e) = (h k l) \cdot R^{-1}$$

and $(h^e k^e l^e)$ is a plane symmetry related to $(h k l)$. Therefore:

Point symmetry in reciprocal space

$$R^* = R^{-1}$$

Point symmetry transformation in reciprocal space

Example:

Three fold axis $3_{[001]}$:

$$(x \ y \ z) \longrightarrow (-y \ x - y \ z) \longrightarrow (y - x \ -x \ z)$$

Point symmetry transformation in reciprocal space

Example:

Three fold axis $3_{[001]}$:

$$(x \ y \ z) \longrightarrow (-y \ x - y \ z) \longrightarrow (y - x \ -x \ z)$$

$$R = \begin{pmatrix} 0 & \bar{1} & 0 \\ 1 & \bar{1} & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

Point symmetry transformation in reciprocal space

Example:

Three fold axis $3_{[001]}$:

$$(x y z) \longrightarrow (-y \ x - y \ z) \longrightarrow (y - x \ -x \ z)$$

$$R = \begin{pmatrix} 0 & \bar{1} & 0 \\ 1 & \bar{1} & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$R^* = \begin{pmatrix} \bar{1} & 1 & 0 \\ \bar{1} & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

Point symmetry transformation in reciprocal space

Example:

Three fold axis $3_{[001]}$:

$$(x y z) \longrightarrow (-y \ x - y \ z) \longrightarrow (y - x \ -x \ z)$$

$$R = \begin{pmatrix} 0 & \bar{1} & 0 \\ 1 & \bar{1} & 0 \\ 0 & 0 & 1 \end{pmatrix} \qquad R^* = \begin{pmatrix} \bar{1} & 1 & 0 \\ \bar{1} & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$(h k l) \longrightarrow (-h - k \ h \ l) \longrightarrow (k \ -h - k \ l)$$

Symmetry group in reciprocal space

Symmetry group in reciprocal space

$$\{R^*\} = \{R\}$$

Symmetry group in reciprocal space

Grupo espacial $C2/m$

Symmetry operation:

$$x y z$$

$$\bar{x} y \bar{z}$$

$$\bar{x} \bar{y} \bar{z}$$

$$x \bar{y} z$$

Symmetry group in reciprocal space

Grupo espacial $C2/m$

Symmetry operation:

$$x y z$$

$$\bar{x} y \bar{z}$$

$$\bar{x} \bar{y} \bar{z}$$

$$x \bar{y} z$$

Equivalent planes:

$$h k l$$

$$\bar{h} k \bar{l}$$

$$\bar{h} \bar{k} \bar{l}$$

$$h \bar{k} l$$

Symmetry group in reciprocal space

Grupo espacial $P222$

Symmetry operation:

$$x \ y \ z$$

$$\bar{x} \ \bar{y} \ z$$

$$\bar{x} \ y \ \bar{z}$$

$$x \ \bar{y} \ \bar{z}$$

Fourier transform and reciprocal vectors

Fourier transform

$$\Gamma[f(\vec{r})] = \hat{f}(\vec{r}^*) = F(\vec{r}^*) \equiv \int_{-\infty}^{\infty} f(\vec{r}) \exp(-2\pi i \vec{r}^* \cdot \vec{r}) d\vec{r}$$

where

$$\vec{r}^* = x^* \vec{a}^* + y^* \vec{b}^* + z^* \vec{c}^*$$

$$\vec{r} = x \vec{a} + y \vec{b} + z \vec{c}$$

and therefore

$$\vec{r}^* \cdot \vec{r} = x^* x + y^* y + z^* z$$

Fourier transform of the lattice

Definition (Dirac comb)

$$L = \sum_{u,v,w=-\infty}^{\infty} \delta(\vec{r} - u\vec{a} - v\vec{b} - w\vec{c})$$

$$\begin{aligned} \Gamma[L(\vec{r})] &= \int \cdots \int_{-\infty}^{\infty} \sum_{u,v,w=-\infty}^{\infty} \delta(\vec{r} - u\vec{a} - v\vec{b} - w\vec{c}) \exp(-2\pi i \vec{r}^* \cdot \vec{r}) d\vec{r} \\ &= \sum_{u,v,w=-\infty}^{\infty} \exp(-2\pi i \vec{r}^* \cdot (u\vec{a} + v\vec{b} + w\vec{c})) \\ &= \sum_{u=-\infty}^{\infty} e^{(-2\pi i u \vec{r}^* \cdot \vec{a})} \sum_{v=-\infty}^{\infty} e^{(-2\pi i v \vec{r}^* \cdot \vec{b})} \sum_{w=-\infty}^{\infty} e^{(-2\pi i w \vec{r}^* \cdot \vec{c})} \end{aligned}$$

Fourier transform of the lattice

Dirac comb

$$\frac{1}{|a|} \sum_{n=-\infty}^{\infty} \exp(2\pi i n x / a) = \sum_{m=-\infty}^{\infty} \delta(x - ma)$$

Fourier transform of the lattice

Dirac comb

$$\frac{1}{|a|} \sum_{n=-\infty}^{\infty} \exp(2\pi i n x / a) = \sum_{m=-\infty}^{\infty} \delta(x - ma)$$

$$\Gamma[L(\vec{r})] = \sum_{u=-\infty}^{\infty} e^{(-2\pi i u \vec{r}^* \cdot \vec{a})} \sum_{v=-\infty}^{\infty} e^{(-2\pi i v \vec{r}^* \cdot \vec{b})} \sum_{w=-\infty}^{\infty} e^{(-2\pi i w \vec{r}^* \cdot \vec{c})}$$

Fourier transform of the lattice

Dirac comb

$$\frac{1}{|a|} \sum_{n=-\infty}^{\infty} \exp(2\pi i n x / a) = \sum_{m=-\infty}^{\infty} \delta(x - ma)$$

$$\Gamma[L(\vec{r})] = \sum_{u=-\infty}^{\infty} e^{(-2\pi i u \vec{r}^* \cdot \vec{a})} \sum_{v=-\infty}^{\infty} e^{(-2\pi i v \vec{r}^* \cdot \vec{b})} \sum_{w=-\infty}^{\infty} e^{(-2\pi i w \vec{r}^* \cdot \vec{c})}$$

$$\begin{aligned} L^*(\vec{r}^*) &= \sum_{h,k,l=-\infty}^{\infty} \delta(\vec{r}^* \cdot \vec{a} - h) \delta(\vec{r}^* \cdot \vec{b} - k) \delta(\vec{r}^* \cdot \vec{c} - l) \\ &= \sum_{h,k,l=-\infty}^{\infty} \delta(\vec{r}^* - h\vec{a}^*) \delta(\vec{r}^* - k\vec{b}^*) \delta(\vec{r}^* - l\vec{c}^*) \end{aligned}$$