

Reciprocal Lattice

Hammond - Chapter 6, A5
 Krawitz - Chapter 2.8, 2.9, 2.10
 Sherwood & Cooper - Chapter 8.7 (page 269 ~ 274; < 6 pages)
 Cullity - Chapter 2-4, A1-1, A1-2, A1-3
 Ott - Chapter 13.3

RL is used to understand
 Geometry of X-ray and electron diffraction
 Behavior of electrons in crystals

Basic concept & application of reciprocal lattice to the analysis of XRD pattern ← P. P. Ewald

[uvw] & (hkl)

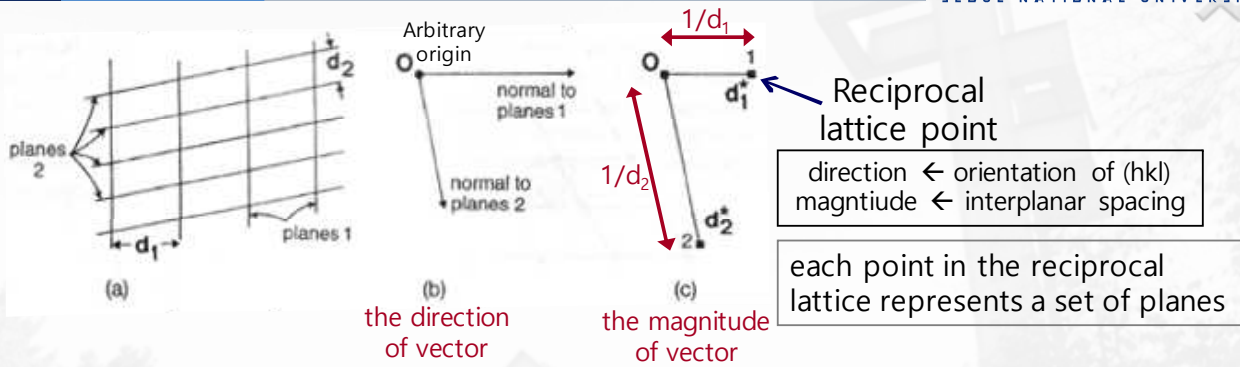
[uvw] (1) a lattice line through the origin and point uvw
 (2) the infinite set of lattice lines which are parallel to it and have the same lattice parameter

(hkl) an infinite set of parallel planes with a constant interplanar spacing

an infinite set of parallel planes which are apart from each other by the **same distance**

interplanar spacing d_{hkl}

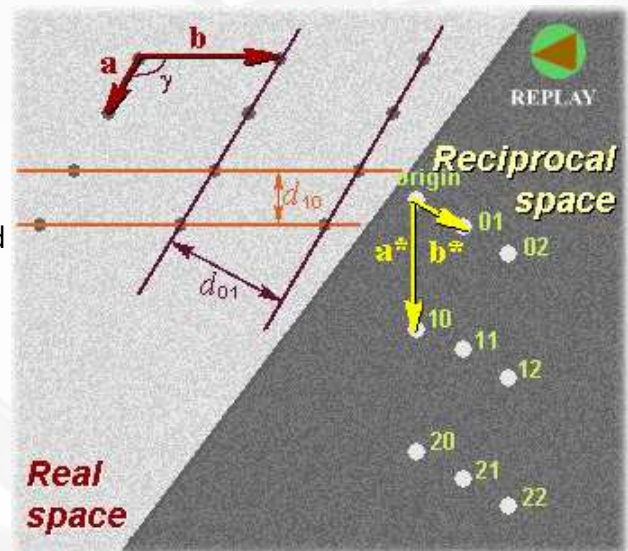
Reciprocal lattice



- Used to understand
 - ✓ the information in a diffraction pattern
 - ✓ many useful geometric calculations to be performed in crystallography
 - ✓ geometry of X-ray and electron diffraction
 - ✓ behavior of electrons in crystals
- Basic concept & application of reciprocal lattice to the analysis of XRD pattern ← P. P. Ewald

2D reciprocal lattice

- For every real lattice, there is an equivalent reciprocal lattice (RL).
- A 2-D real lattice is defined by two unit cell vectors, \vec{a} and \vec{b} inclined at an angle γ .
- The equivalent RL in reciprocal space is defined by two RL vectors, \vec{a}^* and \vec{b}^* .
 - ✓ magnitude of $\vec{a}^* = 1/d_{10}$ and $\vec{a}^* \perp \vec{b}$
(d_{10} = interplanar spacing of (10) planes)
 - ✓ magnitude of $\vec{b}^* = 1/d_{01}$ and $\vec{b}^* \perp \vec{a}$
(d_{01} = interplanar spacing of (01) planes)

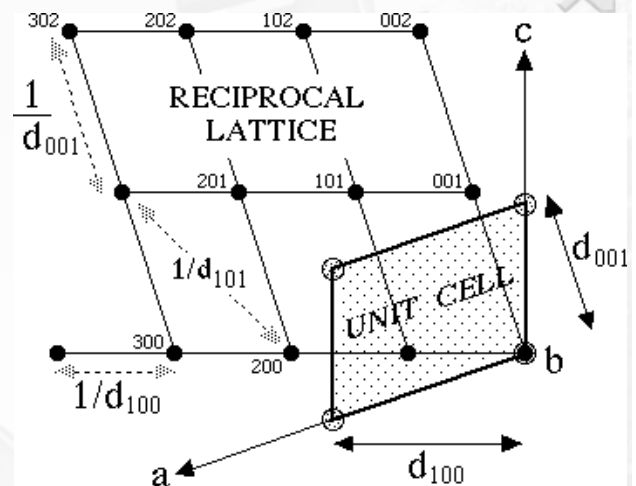


- A RL can be built using RL vectors.
- Both the real and reciprocal constructions show the same lattice, using different but equivalent descriptions.

www4.hcmut.edu.vn/~huynhqlinh/project/Minhhoa3/Nhieuxa/Nx2/www.matter.org.uk/diffraction/geometry/2D_reciprocal_lattices.htm

3D reciprocal lattice

- In a crystal of any structure, RL vector \vec{r}^* is \perp to (hkl) plane and has a length **inversely** proportional to d_{hkl} .



- Why do we need the concept of reciprocal lattice?
 - ✓ A family of planes can be represented by just one point, which obviously simplifies things.
 - ✓ It offers us a very simple geometric model that can interpret the diffraction phenomena in crystals.

http://www4.hcmut.edu.vn/~huynhqlinh/project/Minhhoa3/Nhieuxa/Nx2/www.matter.org.uk/diffraction/geometry/2D_reciprocal_lattices.htm

CHAN PARK, MSE, SNU Spring-2022 Crystal Structure Analyses

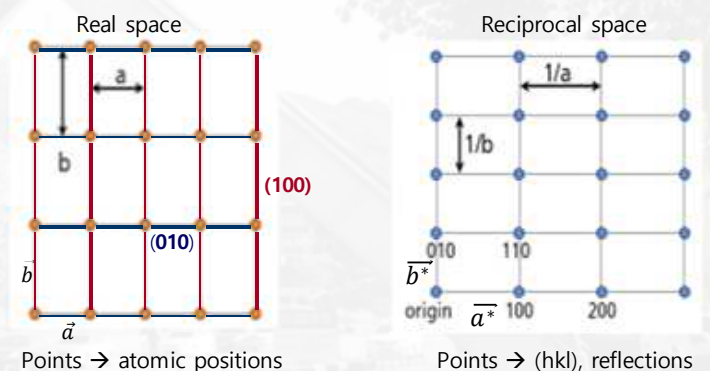
<https://www.xtal.iqfr.csic.es/Cristalografia/index-en.html>

5

What is the reciprocal lattice?

- When we need to consider certain planes in a crystal structure, it is more convenient to use **surface normals** rather than two-dimensional crystal planes.
- In the stereographic projection, a pole (which represent a set of crystal planes) can be described by a point.
- In the stereographic projection, the relative position of the planes and interplanar angles can be determined from the relative position of the poles. But the interplanar spacing (d), which is needed to determine the position of the diffracted X-ray (the θ in Bragg's law), cannot be obtained from the relative position of the poles.

- Reciprocal lattice includes information on both the relative position of the planes and the interplanar spacing.

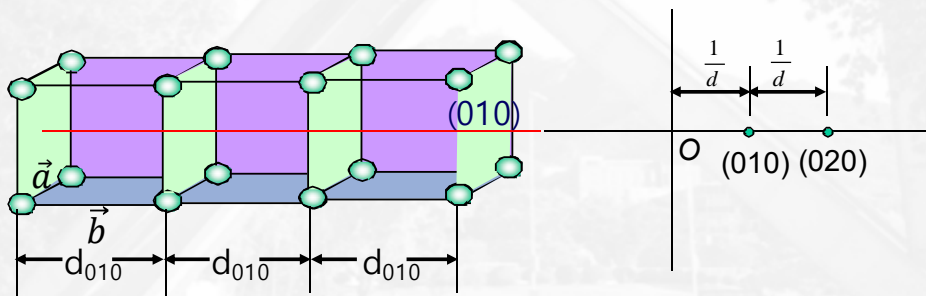


Points \rightarrow atomic positions

Points \rightarrow (hkl), reflections

What is the reciprocal lattice?

- Families of planes in crystals can be represented simply by their normal, which are then specified as (reciprocal lattice (RL)) vectors.
- RL vectors can be used to define a pattern of (RL) points, each (RL) point representing a family of planes.
- Advantage ; RL accentuates the connections between families of planes in the crystals, Bragg's law and the directions of the diffracted or reflected beams.



Reciprocal lattice

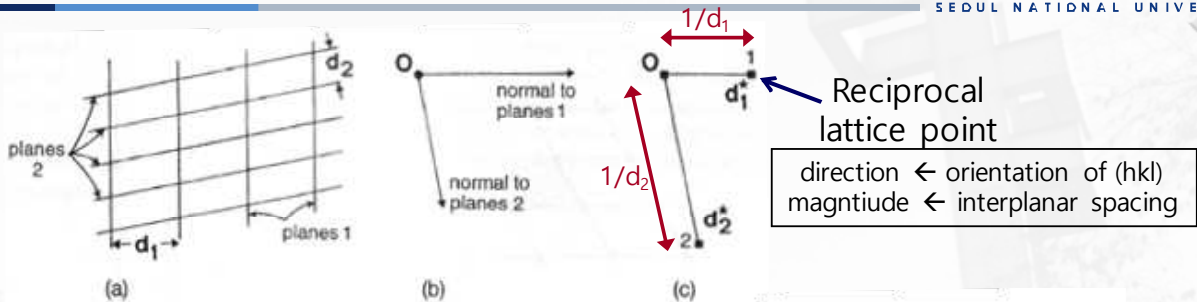


Fig. 6.1. (a) Traces of two families of planes 1 and 2 (perpendicular to the plane of the paper), (b) the normals to these families of planes drawn from a common origin and (c) definition of these planes in terms of the reciprocal (lattice) vectors d_1^* and d_2^* , where $d_1^* = K/d_1$, $d_2^* = K/d_2$, K being a constant.

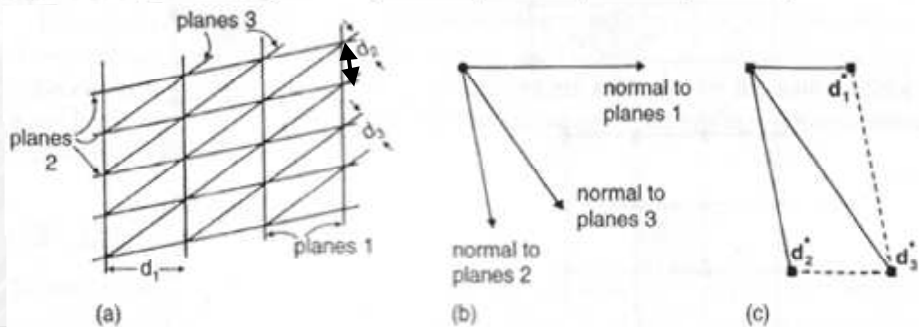
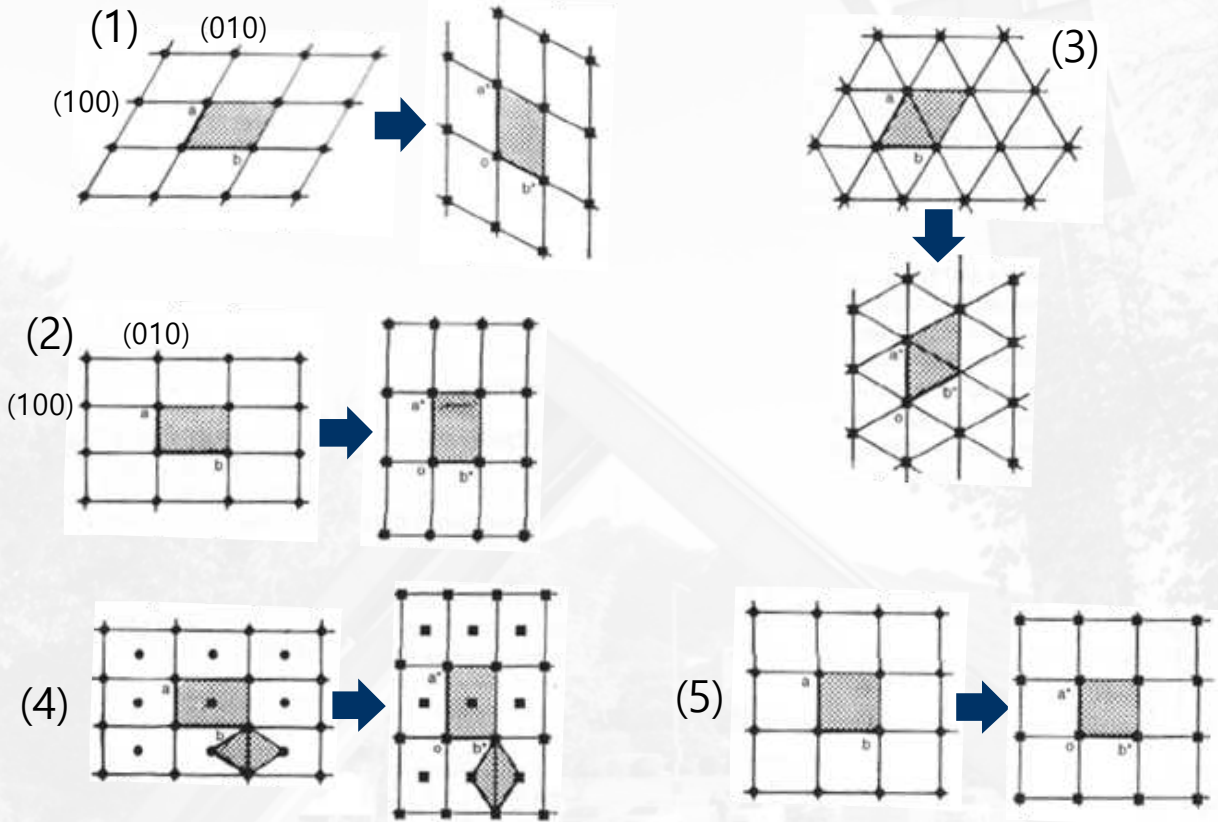


Fig. 6.2. As Fig. 6.1, showing in Fig. 6.2(a) a third set of intersecting planes (planes 3), their normals in Fig. 6.2(b) and their reciprocal lattice vectors in Fig. 6.2(c). Note that $d_1^* + d_2^* = d_3^*$ and that the reciprocal lattice points do form a lattice.

5 plane lattices and their reciprocal lattices



Real vs. reciprocal lattice

Fig. 8.7. The unit cells of a real and reciprocal lattice. Note that a^* is perpendicular to the plane of b and c ; and similarly for b^* and c^* . For clarity, the two figures are not drawn to scale.

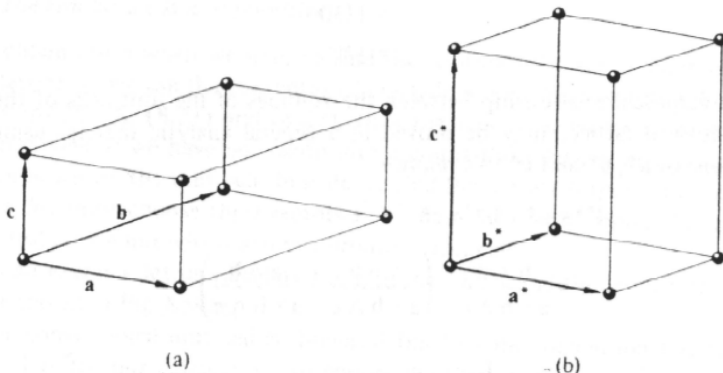
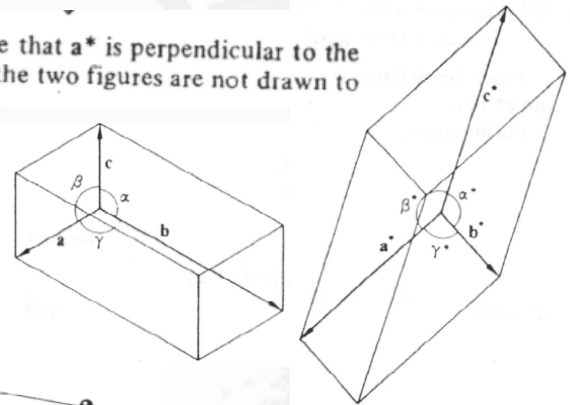
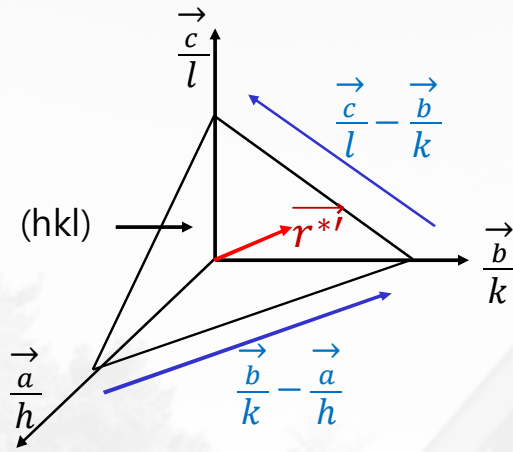


Fig. 8.8. The reciprocal lattice of a primitive orthorhombic real lattice. The reciprocal lattice is also primitive orthorhombic. For clarity, (b) is drawn on a larger scale than (a).



$$\begin{aligned} \vec{r}^* &= \left(\frac{\vec{b}}{k} - \frac{\vec{a}}{h} \right) \times \left(\frac{\vec{c}}{l} - \frac{\vec{b}}{k} \right) \\ &= \frac{\vec{b} \times \vec{c}}{kl} + \frac{\vec{c} \times \vec{a}}{lh} + \frac{\vec{a} \times \vec{b}}{hk} \\ &= \frac{abc}{hkl} \left(h \frac{\vec{b} \times \vec{c}}{abc} + k \frac{\vec{c} \times \vec{a}}{abc} + l \frac{\vec{a} \times \vec{b}}{abc} \right) \end{aligned}$$

$$\vec{r}^* = h \frac{\vec{b} \times \vec{c}}{abc} + k \frac{\vec{c} \times \vec{a}}{abc} + l \frac{\vec{a} \times \vec{b}}{abc} = h\vec{a}^* + k\vec{b}^* + l\vec{c}^* \quad abc = \vec{a} \cdot \vec{b} \times \vec{c}$$

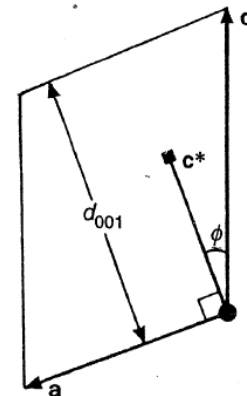
$$\vec{a}^* = \frac{\vec{b} \times \vec{c}}{abc} \quad \vec{b}^* = \frac{\vec{c} \times \vec{a}}{abc} \quad \vec{c}^* = \frac{\vec{a} \times \vec{b}}{abc}$$

$$\begin{aligned} \vec{a} \cdot \vec{a}^* &= 1 & \vec{a} \cdot \vec{b}^* &= 0 & \vec{a} \cdot \vec{c}^* &= 0 \\ \vec{b} \cdot \vec{a}^* &= 0 & \vec{b} \cdot \vec{b}^* &= 1 & \vec{b} \cdot \vec{c}^* &= 0 \\ \vec{c} \cdot \vec{a}^* &= 0 & \vec{c} \cdot \vec{b}^* &= 0 & \vec{c} \cdot \vec{c}^* &= 1 \end{aligned}$$

a, b, c vs. a*, b*, c*

$$\vec{a}^* = \frac{\vec{b} \times \vec{c}}{abc} \quad \vec{b}^* = \frac{\vec{c} \times \vec{a}}{abc} \quad \vec{c}^* = \frac{\vec{a} \times \vec{b}}{abc}$$

$$\begin{aligned} \vec{a} \cdot \vec{a}^* &= 1 & \vec{a} \cdot \vec{b}^* &= 0 & \vec{a} \cdot \vec{c}^* &= 0 \\ \vec{b} \cdot \vec{a}^* &= 0 & \vec{b} \cdot \vec{b}^* &= 1 & \vec{b} \cdot \vec{c}^* &= 0 \\ \vec{c} \cdot \vec{a}^* &= 0 & \vec{c} \cdot \vec{b}^* &= 0 & \vec{c} \cdot \vec{c}^* &= 1 \end{aligned}$$



Since \vec{c}^* is perpendicular to both \vec{a} and \vec{b} , the scalar (or dot) products are zero, i.e. $\vec{c}^* \cdot \vec{a} = 0$, $\vec{c}^* \cdot \vec{b} = 0$ and similarly for \vec{a}^* and \vec{b}^* , i.e. $\vec{a}^* \cdot \vec{b} = 0$, $\vec{a}^* \cdot \vec{c} = 0$, $\vec{b}^* \cdot \vec{a} = 0$, $\vec{b}^* \cdot \vec{c} = 0$.

Now consider the scalar product $\vec{c} \cdot \vec{c}^* = c|\vec{c}^*| \cos \phi$. However, since $|\vec{c}^*| = 1/d_{001}$ by definition and $c \cos \phi = d_{001}$, then $\vec{c} \cdot \vec{c}^* = d_{001}/d_{001} = 1$ and similarly for $\vec{a} \cdot \vec{a}^* = 1$ and $\vec{b} \cdot \vec{b}^* = 1$.

$$\begin{aligned} \vec{a}^* &\perp (100), \text{ magnitude} = 1/d_{100} \\ \vec{b}^* &\perp (010), \text{ magnitude} = 1/d_{010} \\ \vec{c}^* &\perp (001), \text{ magnitude} = 1/d_{001} \end{aligned}$$

b_1, b_2, b_3 ; reciprocal lattice

$$b_1 = \frac{a_2 \times a_3}{a_1 \cdot a_2 \times a_3}$$

$$b_2 = \frac{a_3 \times a_1}{a_1 \cdot a_2 \times a_3}$$

$$b_3 = \frac{a_1 \times a_2}{a_1 \cdot a_2 \times a_3}$$

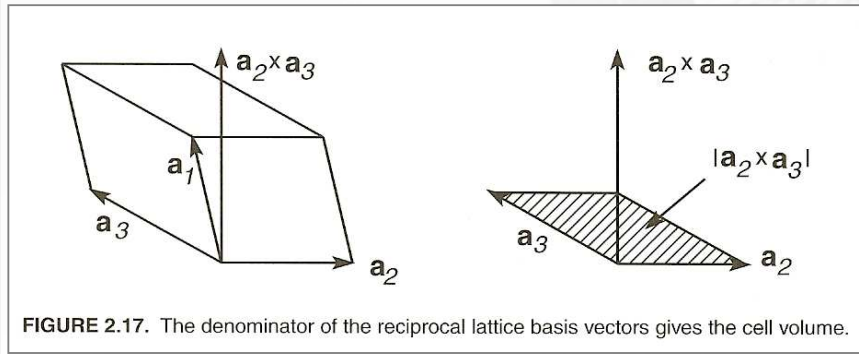


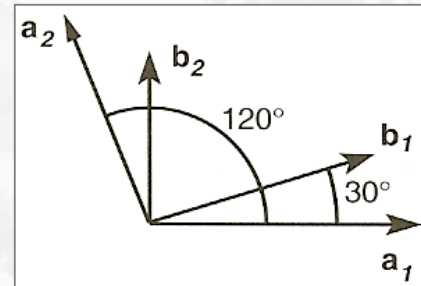
FIGURE 2.17. The denominator of the reciprocal lattice basis vectors gives the cell volume.

$$a_i \cdot b_i = 1$$

$$b_i \cdot a_j = 0, \quad \text{for } i \neq j$$

$$a_1 \cdot b_1 = a_1 \times |b_1| \times \cos(\text{angle})$$

$$= a_1 \times 1/d_{001} \times d_{001}/a_1 = 1$$



Reciprocal Lattice of a monoclinic P

$$a \neq b \neq c \quad \alpha = \gamma = 90^\circ \neq \beta$$

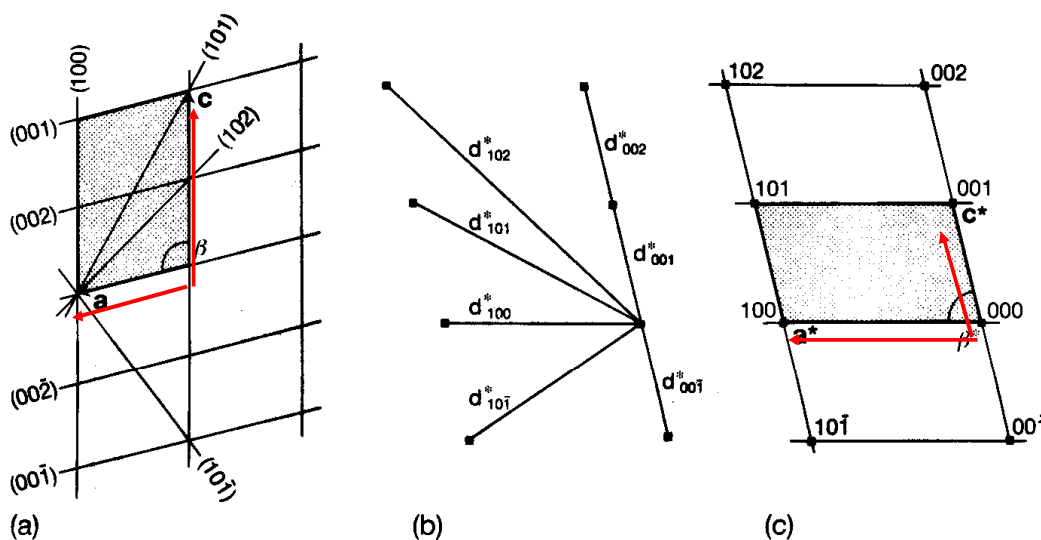
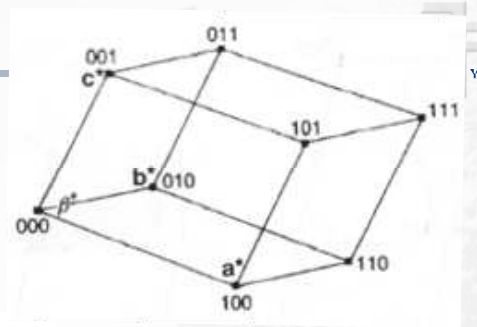


Fig 6.4 (a) Plan of a monoclinic P unit cell perpendicular to the y -axis with the unit cell shaded. The traces of some planes of type $\{h0l\}$ (i.e. parallel to the y -axis) are indicated, (b) the reciprocal (lattice) vectors, d_{hkl}^* for these planes and (c) the reciprocal lattice defined by these vectors. Each reciprocal lattice point is labelled with the indices of the plane it represents and the unit cell is shaded. The angle β^* is the complement of β .

Reciprocal Lattice of a monoclinic P



Reciprocal lattice unit cell of a monoclinic P crystal

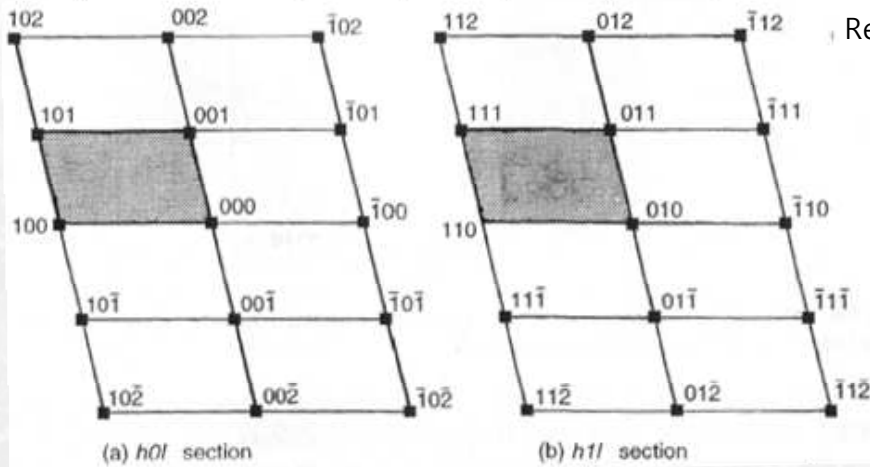


Fig. 6.5. Sections of a monoclinic reciprocal lattice perpendicular to the \mathbf{b}^* vector or y^* -axis. (a) $h0l$ section through the origin 000 , built up by simply extending the section in Fig. 6.4(c); (b) $h1l$ section (representing planes intersecting the y -axis at one lattice vector \mathbf{b}) 'one layer up' along the \mathbf{b}^* axis.

Reciprocal Lattice

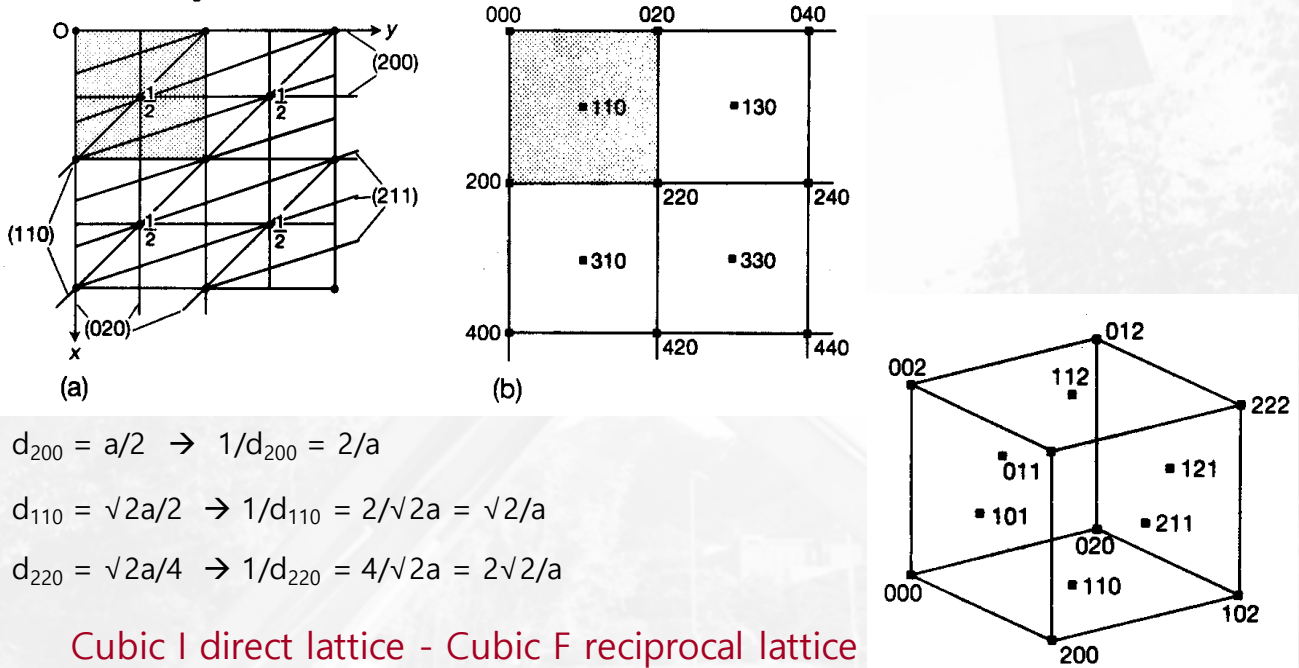
- Direction symbols $[uvw]$ are the components of a vector \mathbf{r}_{uvw} in direct space (direct lattice vector).

$$\mathbf{r}_{uvw} = u\mathbf{a} + v\mathbf{b} + w\mathbf{c}$$

- Laue indices are simply the components of a reciprocal lattice vector.

$$\mathbf{d}_{hkl}^* = h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c}^*$$

Fig. 6.4. (a) Plan of a cubic *I* crystal perpendicular to the *z*-axis and (b) pattern of reciprocal lattice points perpendicular to the *z*-axis. Note the cubic *F* arrangement of reciprocal lattice points in this plane.



$$d_{200} = a/2 \rightarrow 1/d_{200} = 2/a$$

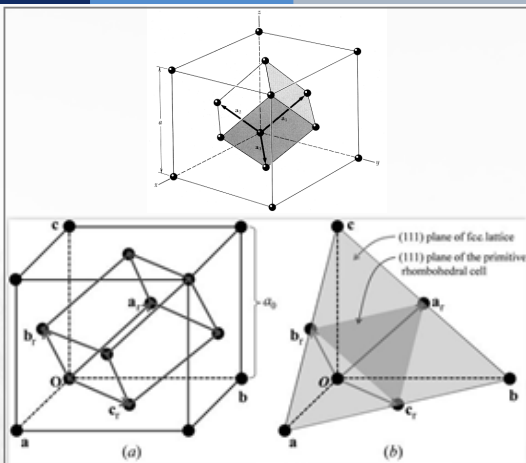
$$d_{110} = \sqrt{2}a/2 \rightarrow 1/d_{110} = 2/\sqrt{2}a = \sqrt{2}/a$$

$$d_{220} = \sqrt{2}a/4 \rightarrow 1/d_{220} = 4/\sqrt{2}a = 2\sqrt{2}/a$$

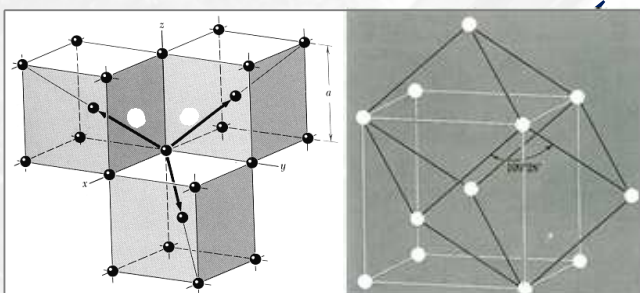
Cubic *I* direct lattice - Cubic *F* reciprocal lattice

Cubic *F* direct lattice - Cubic *I* reciprocal lattice

Real vs Reciprocal lattice in Cubic

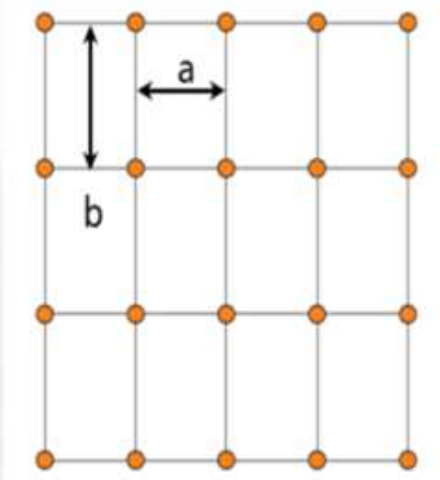


Real space	Reciprocal space
Cubic <i>F</i> (rhombohedral 60°)	Cubic <i>I</i> (rhombohedral 109.47°)
Cubic <i>P</i> (rhombohedral 90°)	Cubic <i>P</i> (rhombohedral 90°)
Cubic <i>I</i> (rhombohedral 109.47°)	Cubic <i>F</i> (rhombohedral 60°)



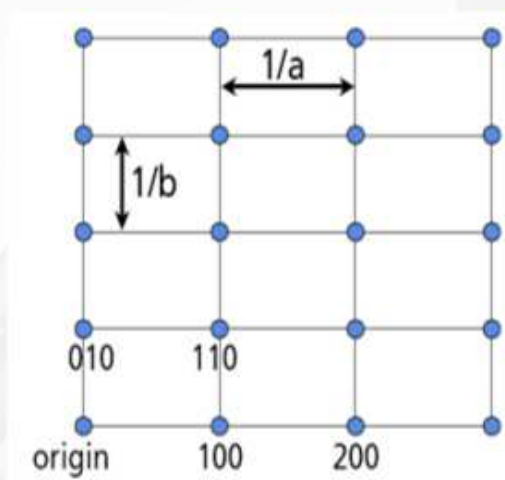
Real lattice $\xleftrightarrow{\text{Fourier transform}}$ Reciprocal lattice

Real space



Points → atomic positions

Reciprocal space

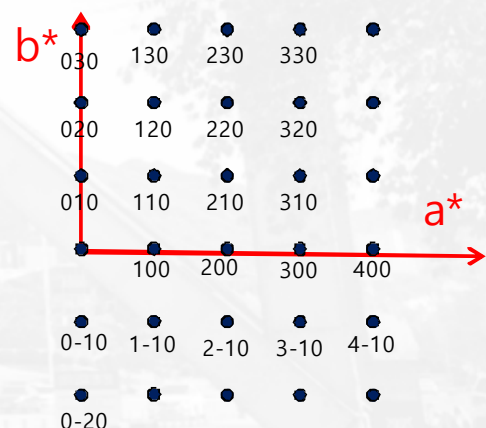
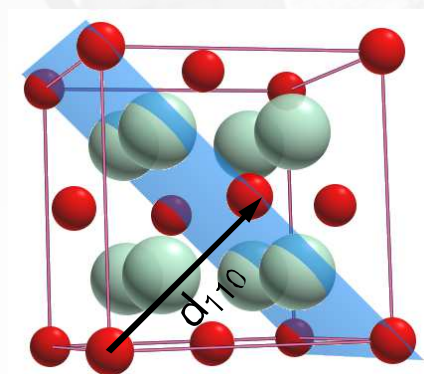


Points → (hkl), reflections

Reciprocal lattice

- d_{hkl} is the vector drawn from the origin of the unit cell to intersect the first crystallographic plane in the family (hkl) at a 90° angle.
- The reciprocal vector is d^*_{hkl} , $|d^*_{hkl}| = 1/d_{hkl}$.
- In the reciprocal lattice, each point represents a vector which, in turn, represents a set of Bragg planes.
- Each reciprocal vector can be resolved into the components:

$$d^*_{hkl} = ha^* + kb^* + lc^*$$



Reciprocal lattice vector \mathbf{r}_{hkl}^* is normal to real lattice plane (hkl) .

$$\mathbf{r}_{hkl}^* \perp (hkl)$$

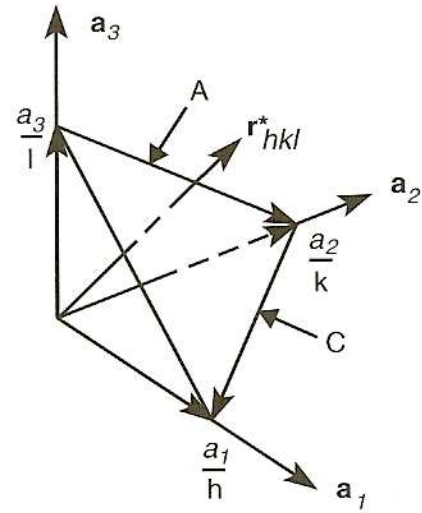
$$\mathbf{A} = \frac{\mathbf{a}_2}{k} - \frac{\mathbf{a}_3}{l}$$

and

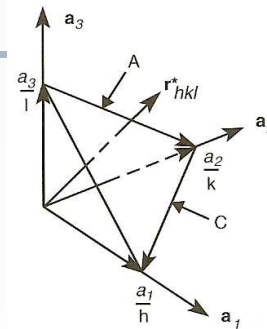
$$\mathbf{C} = \frac{\mathbf{a}_1}{h} - \frac{\mathbf{a}_2}{k}$$

Thus

$$\begin{aligned} \mathbf{A} \cdot \mathbf{r}_{hkl}^* &= \left(\frac{\mathbf{a}_2}{k} - \frac{\mathbf{a}_3}{l} \right) \cdot (h\mathbf{b}_1 + k\mathbf{b}_2 + l\mathbf{b}_3) \\ &= \left(\frac{\mathbf{a}_2}{k} \right) \cdot (h\mathbf{b}_1 + k\mathbf{b}_2 + l\mathbf{b}_3) - \left(\frac{\mathbf{a}_3}{l} \right) \cdot (h\mathbf{b}_1 + k\mathbf{b}_2 + l\mathbf{b}_3) \\ &= \left(0 + \frac{k}{k} + 0 \right) - \left(0 + 0 + \frac{l}{l} \right) \\ &= 0. \quad \rightarrow \mathbf{A} \perp \mathbf{r}_{hkl}^* \quad \& \quad \mathbf{C} \perp \mathbf{r}_{hkl}^* \rightarrow \mathbf{r}_{hkl}^* \perp (hkl) \end{aligned}$$



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

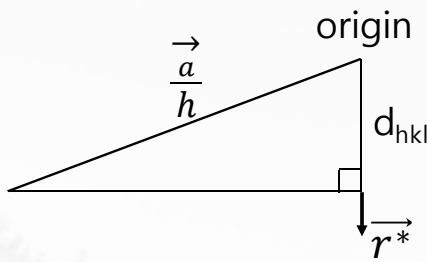


The magnitude of \mathbf{r}_{hkl}^* is the inverse of the interplanar spacing of the (hkl) planes, d_{hkl} . The unit normal to (hkl) is given by $\mathbf{n} = \mathbf{r}_{hkl}^* / |\mathbf{r}_{hkl}^*|$ so that $\mathbf{n} = (h\mathbf{b}_1 + k\mathbf{b}_2 + l\mathbf{b}_3) / |\mathbf{r}_{hkl}^*|$. Referring again to Figure 2.18, the projection of \mathbf{a}_1/h onto \mathbf{n} gives d_{hkl} so

$$d_{hkl} = \frac{\mathbf{a}_1}{h} \cdot \mathbf{n} = \frac{\mathbf{a}_1}{h} \cdot \frac{h\mathbf{b}_1 + k\mathbf{b}_2 + l\mathbf{b}_3}{|\mathbf{r}_{hkl}^*|} = \frac{1}{|\mathbf{r}_{hkl}^*|}$$

Thus the inverse of the magnitude of the reciprocal lattice vector \mathbf{r}_{hkl}^* is equal to the interplanar spacing of the (hkl) of the real lattice, and

$$|\mathbf{r}_{hkl}^*| = \frac{1}{d_{hkl}} \quad (2.6)$$



$$d_{hkl} = \frac{\vec{a}}{h} \cdot \frac{\vec{r}^*}{|\vec{r}^*|} = \frac{\vec{a}}{h} \cdot \frac{h\vec{a}^* + k\vec{b}^* + l\vec{c}^*}{|\vec{r}^*|} = \frac{1}{|\vec{r}^*|}$$

$$r_{hkl}^2 = \frac{1}{d_{hkl}^2} = (h\vec{a}^* + k\vec{b}^* + l\vec{c}^*) \cdot (h\vec{a}^* + k\vec{b}^* + l\vec{c}^*)$$

$$= h^2 a^{*2} + k^2 b^{*2} + l^2 c^{*2} + 2a^* b^* \cos \gamma^* + 2b^* c^* \cos \alpha^* + 2c^* a^* \cos \beta^*$$

For cubic, $a=b=c$, $\alpha=\beta=\gamma=90^\circ$, $a^*=b^*=c^*=1/a$, $\alpha^*=\beta^*=\gamma^*=90^\circ$, $a^* \cdot a^* = 1/a^2$

$$r_{hkl}^2 = \frac{1}{d_{hkl}^2} = \frac{h^2 + k^2 + l^2}{a^2} \quad d_{hkl} = \frac{a}{\sqrt{h^2 + k^2 + l^2}} \quad \text{Cubic}$$

Interplanar spacing

$$|\vec{r}_{hkl}^*|^2 = \frac{1}{d_{hkl}^2} = (h\mathbf{b}_1 + k\mathbf{b}_2 + l\mathbf{b}_3) \cdot (h\mathbf{b}_1 + k\mathbf{b}_2 + l\mathbf{b}_3)$$

$$= h^2 \mathbf{b}_1 \cdot \mathbf{b}_1 + k^2 \mathbf{b}_2 \cdot \mathbf{b}_2 + l^2 \mathbf{b}_3 \cdot \mathbf{b}_3 + 2hk \mathbf{b}_1 \cdot \mathbf{b}_2 + 2kl \mathbf{b}_2 \cdot \mathbf{b}_3 + 2hl \mathbf{b}_3 \cdot \mathbf{b}_1$$

Expanding the \mathbf{b}_i in terms of their real space definitions, and factoring out the denominator, we have

$$= \frac{1}{V^2} \{ h^2 |\mathbf{a}_2 \times \mathbf{a}_3|^2 + k^2 |\mathbf{a}_3 \times \mathbf{a}_1|^2 + l^2 |\mathbf{a}_1 \times \mathbf{a}_2|^2 + 2hk (\mathbf{a}_2 \times \mathbf{a}_3) \cdot (\mathbf{a}_3 \times \mathbf{a}_1) + 2kl (\mathbf{a}_3 \times \mathbf{a}_1) \cdot (\mathbf{a}_1 \times \mathbf{a}_2) + 2hl (\mathbf{a}_1 \times \mathbf{a}_2) \cdot (\mathbf{a}_2 \times \mathbf{a}_3) \}$$

Two results from vector algebra are used to simplify this expression:

$$|\mathbf{a}_i \times \mathbf{a}_j|^2 = a_i^2 a_j^2 \sin^2 \alpha_{ij}$$

$$(\mathbf{a}_i \times \mathbf{a}_j) \cdot (\mathbf{a}_j \times \mathbf{a}_k) = (\mathbf{a}_i \cdot \mathbf{a}_j)(\mathbf{a}_j \cdot \mathbf{a}_k) - \mathbf{a}_i \cdot \mathbf{a}_k a_j^2$$

This enables the final result:

$$\frac{1}{d_{hkl}^2} = \frac{a_1^2 a_2^2 a_3^2}{V^2} \left[\frac{h^2 \sin^2 \alpha}{a_1^2} + \frac{k^2 \sin^2 \beta}{a_2^2} + \frac{l^2 \sin^2 \gamma}{a_3^2} + \frac{2hk}{a_1 a_2} (\cos \alpha \cos \beta - \cos \gamma) + \frac{2kl}{a_2 a_3} (\cos \beta \cos \gamma - \cos \alpha) + \frac{2lh}{a_1 a_3} (\cos \gamma \cos \alpha - \cos \beta) \right] \quad (2.9)$$

Interplanar spacing

$$d_{hkl}$$

$$\text{Cubic: } \frac{1}{d^2} = \frac{h^2 + k^2 + l^2}{a^2}$$

$$\text{Tetragonal: } \frac{1}{d^2} = \frac{h^2 + k^2}{a^2} + \frac{l^2}{c^2}$$

$$\text{Hexagonal: } \frac{1}{d^2} = \frac{4}{3} \left(\frac{h^2 + hk + k^2}{a^2} \right) + \frac{l^2}{c^2}$$

Rhombohedral:

$$\frac{1}{d^2} = \frac{(h^2 + k^2 + l^2)\sin^2 \alpha + 2(hk + kl + hl)(\cos^2 \alpha - \cos \alpha)}{a^2(1 - 3\cos^2 \alpha + 2\cos^3 \alpha)}$$

$$\text{Orthorhombic: } \frac{1}{d^2} = \frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2}$$

$$\text{Monoclinic: } \frac{1}{d^2} = \frac{1}{\sin^2 \beta} \left(\frac{h^2}{a^2} + \frac{k^2 \sin^2 \beta}{b^2} + \frac{l^2}{c^2} - \frac{2hl \cos \beta}{ac} \right)$$

$$\text{Triclinic: } \frac{1}{d^2} = \frac{1}{V^2} (S_{11}h^2 + S_{22}k^2 + S_{33}l^2 + 2S_{12}hk + 2S_{23}kl + 2S_{13}hl)$$

In the equation for triclinic crystals,

V = volume of unit cell (see below),

$$S_{11} = b^2c^2\sin^2 \alpha,$$

$$S_{22} = a^2c^2\sin^2 \beta,$$

$$S_{33} = a^2b^2\sin^2 \gamma,$$

$$S_{12} = abc^2(\cos \alpha \cos \beta - \cos \gamma),$$

$$S_{23} = a^2bc(\cos \beta \cos \gamma - \cos \alpha),$$

$$S_{13} = ab^2c(\cos \gamma \cos \alpha - \cos \beta).$$

$$\text{Cubic: } \frac{1}{d^2} = \frac{h^2 + k^2 + l^2}{a^2}$$

$$\text{Tetragonal } \frac{1}{d^2} = \frac{h^2 + k^2}{a^2} + \frac{l^2}{c^2}$$

$$\text{Orthorhombic: } \frac{1}{d^2} = \frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2}$$