Reciprocal Lattice

Read
- 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

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

Reciprocal Lattice

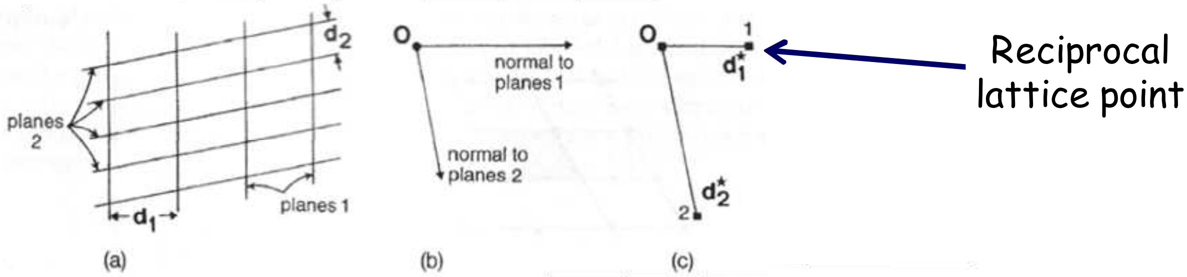

Fig. 6.1. (a) Traces of two families of planes 1 and 2 (perpendicular to the plane of the paper), (b) the normals to these families of planes drawn from a common origin and (c) definition of these planes in terms of the reciprocal (lattice) vectors $\mathbf{d}_1^*$ and $\mathbf{d}_2^*$, where $\mathbf{d}_1^* = K/d_1$, $\mathbf{d}_2^* = K/d_2$, K being a constant.

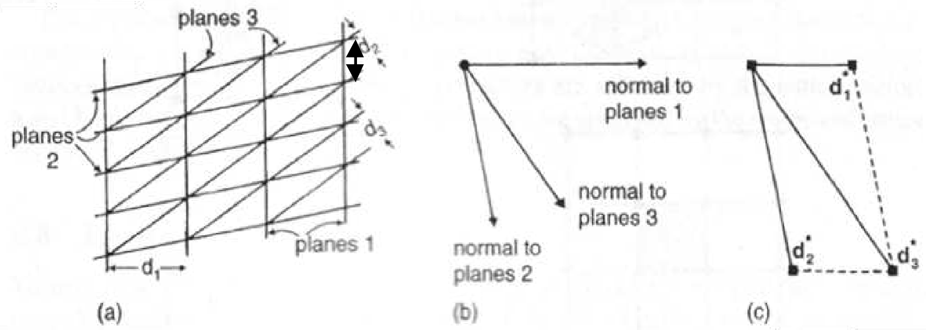

Fig. 6.2. As Fig. 6.1, showing in Fig. 6.2(a) a third set of intersecting planes (planes 3), their normals in Fig. 6.2(b) and their reciprocal lattice vectors in Fig. 6.2(c). Note that $\mathbf{d}_1^* + \mathbf{d}_2^* = \mathbf{d}_3^*$ and that the reciprocal lattice points do form a lattice.

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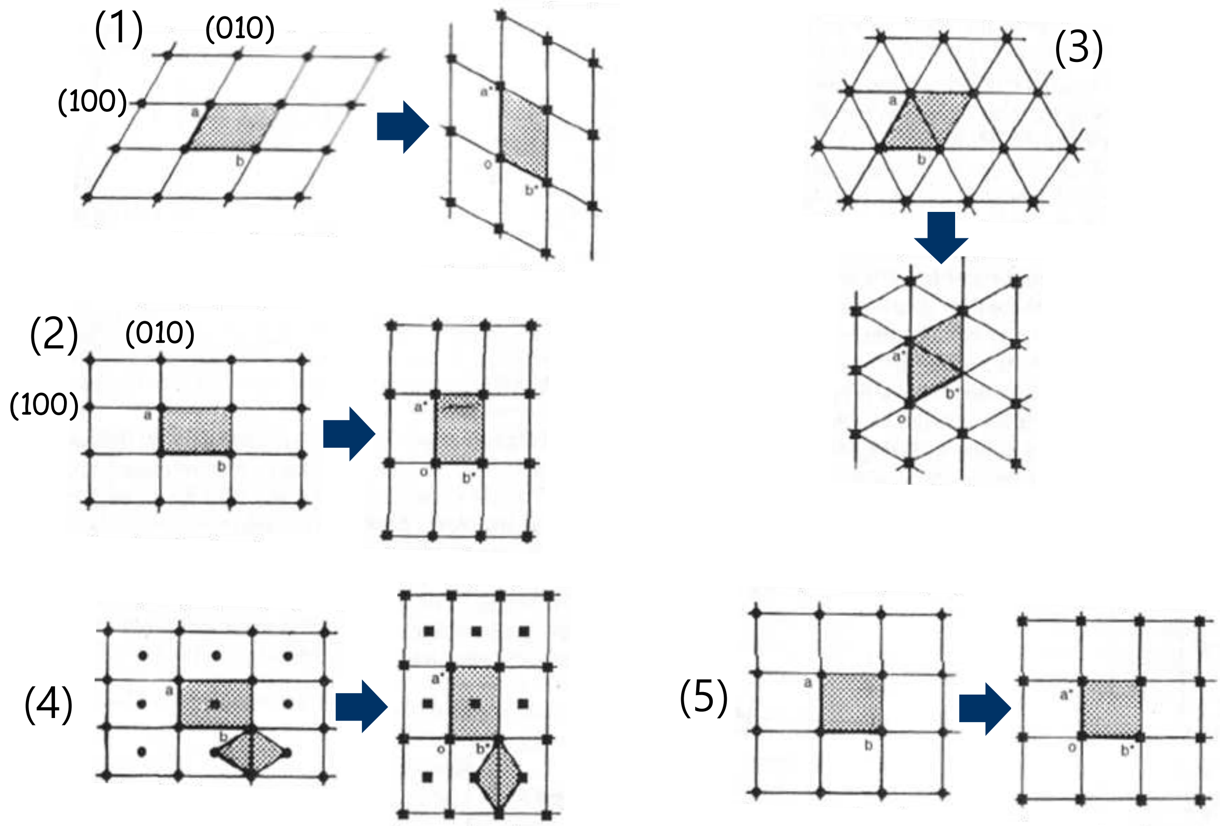
5 plane lattices and their reciprocal lattices



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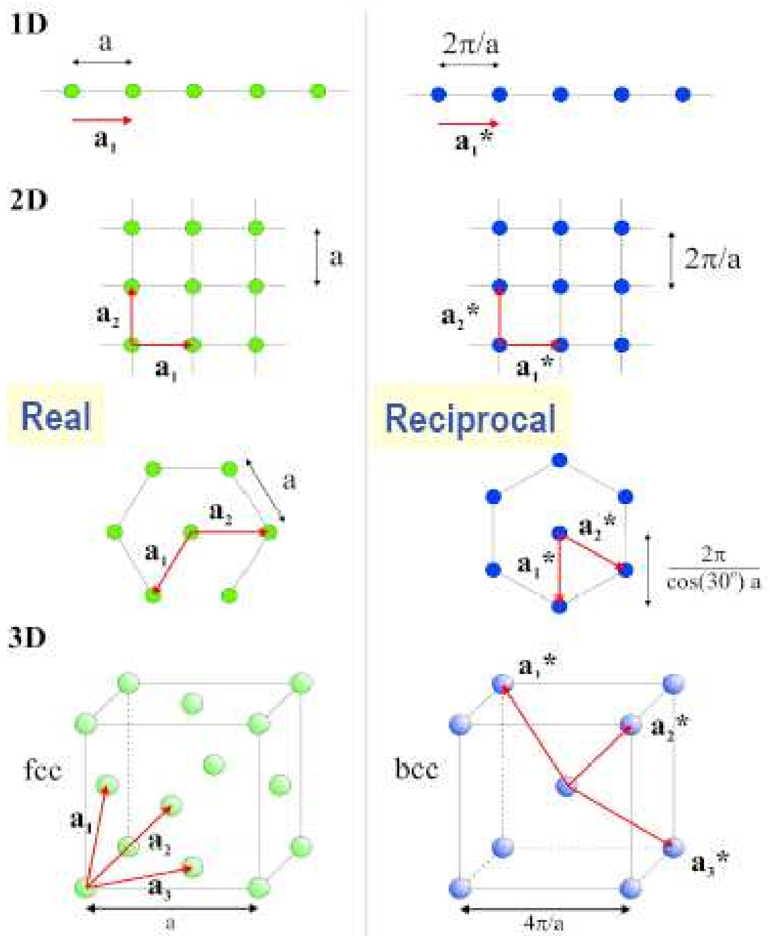


Reciprocal Lattice:

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

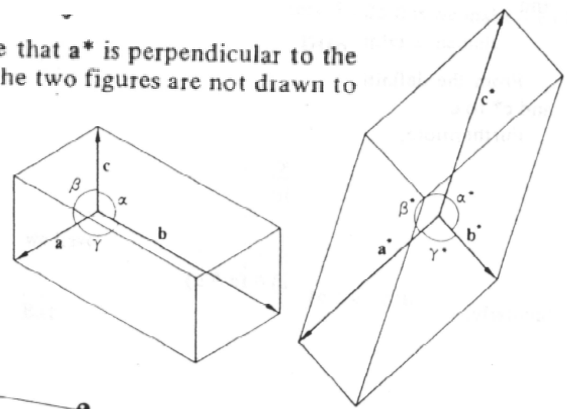
$$\vec{a}_1^* = \frac{2\pi}{V_c} \vec{a}_2 \times \vec{a}_3$$

$$\vec{a}_2^* = \frac{2\pi}{V_c} \vec{a}_3 \times \vec{a}_1$$

$$\vec{a}_3^* = \frac{2\pi}{V_c} \vec{a}_1 \times \vec{a}_2$$

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.



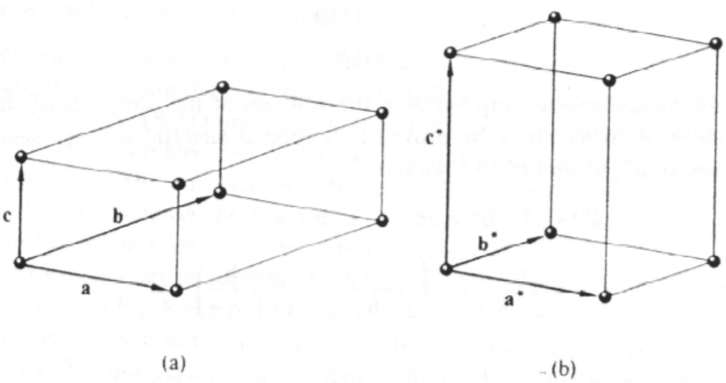
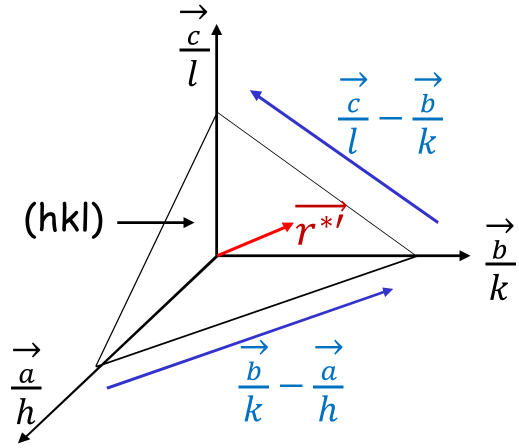


Fig. 8.8. *The reciprocal lattice of a primitive orthorhombic real lattice.* The reciprocal lattice is also primitive orthorhombic. For clarity, (b) is drawn on a larger scale than (a).

 Sherwood & Cooper Chapter 8.7

Reciprocal Lattice



$$\overrightarrow{r^{*\prime}} = \left(\frac{\vec{b}}{k} - \frac{\vec{a}}{h}\right) X \left(\frac{\vec{c}}{l} - \frac{\vec{b}}{k}\right)$$
$$= \frac{\vec{b}\,X\,\vec{c}}{kl} + \frac{\vec{c}\,X\,\vec{a}}{lh} + \frac{\vec{a}\,X\,\vec{b}}{hk}$$
$$= \frac{abc}{hkl}\left(h\frac{\vec{b}\,X\,\vec{c}}{abc} + k\frac{\vec{c}\,X\,\vec{a}}{abc} + l\frac{\vec{a}\,X\,\vec{b}}{abc}\right)$$

$$\overrightarrow{r^*} = h\frac{\vec{b}\,X\,\vec{c}}{abc} + k\frac{\vec{c}\,X\,\vec{a}}{abc} + l\frac{\vec{a}\,X\,\vec{b}}{abc} = h\overrightarrow{a^*} + k\overrightarrow{b^*} + l\overrightarrow{c^*}$$

$$abc = \vec{a}\bullet\vec{b}\,X\,\vec{c}$$

$$\overrightarrow{a^*} = \frac{\vec{b}\,X\,\vec{c}}{abc} \qquad \overrightarrow{b^*} = \frac{\vec{c}\,X\,\vec{a}}{abc} \qquad \overrightarrow{c^*} = \frac{\vec{a}\,X\,\vec{b}}{abc}$$

$\vec{a}\bullet\overrightarrow{a^*} = 1$ $\vec{a}\bullet\overrightarrow{b^*} = 0$ $\vec{a}\bullet\overrightarrow{c^*} = 0$

$\vec{b}\bullet\overrightarrow{a^*} = 0$ $\vec{b}\bullet\overrightarrow{b^*} = 1$ $\vec{b}\bullet\overrightarrow{c^*} = 0$

$\vec{c}\bullet\overrightarrow{a^*} = 0$ $\vec{c}\bullet\overrightarrow{b^*} = 0$ $\vec{c}\bullet\overrightarrow{c^*} = 1$

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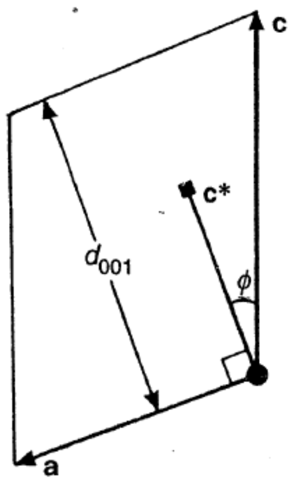
a, b, c vs. a*, b*, c*

$$\overrightarrow{a^*} = \frac{\vec{b}\,X\,\vec{c}}{abc} \qquad \overrightarrow{b^*} = \frac{\vec{c}\,X\,\vec{a}}{abc} \qquad \overrightarrow{c^*} = \frac{\vec{a}\,X\,\vec{b}}{abc}$$

$\vec{a}\bullet\overrightarrow{a^*} = 1$ $\vec{a}\bullet\overrightarrow{b^*} = 0$ $\vec{a}\bullet\overrightarrow{c^*} = 0$

$\vec{b}\bullet\overrightarrow{a^*} = 0$ $\vec{b}\bullet\overrightarrow{b^*} = 1$ $\vec{b}\bullet\overrightarrow{c^*} = 0$

$\vec{c}\bullet\overrightarrow{a^*} = 0$ $\vec{c}\bullet\overrightarrow{b^*} = 0$ $\vec{c}\bullet\overrightarrow{c^*} = 1$



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

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

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Reciprocal lattice

b_1, b_2, b_3; reciprocal lattice

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

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

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

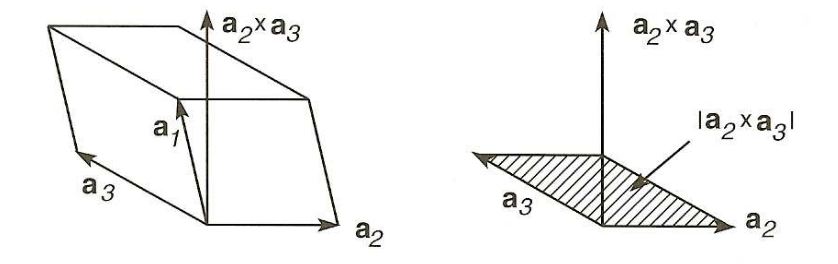
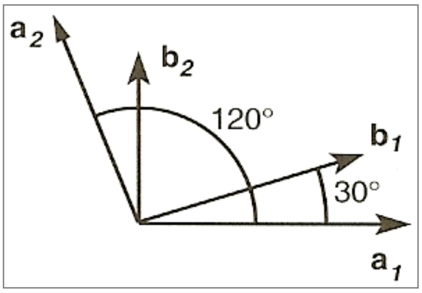


FIGURE 2.17. The denominator of the reciprocal lattice basis vectors gives the cell volume.

$$\mathbf{a}_i \cdot \mathbf{b}_i = 1$$
$$\mathbf{b}_i \cdot \mathbf{a}_j = 0, \qquad \text{for } i \neq j$$



$\mathbf{a_1} \bullet \mathbf{b_1} = a_1 \times |\mathbf{b_1}| \times \cos(\text{angle})$
$= a_1 \times 1/d_{001} \times d_{001}/a_1 = 1$

Krawitz page 64

Reciprocal Lattice of a monoclinic P

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

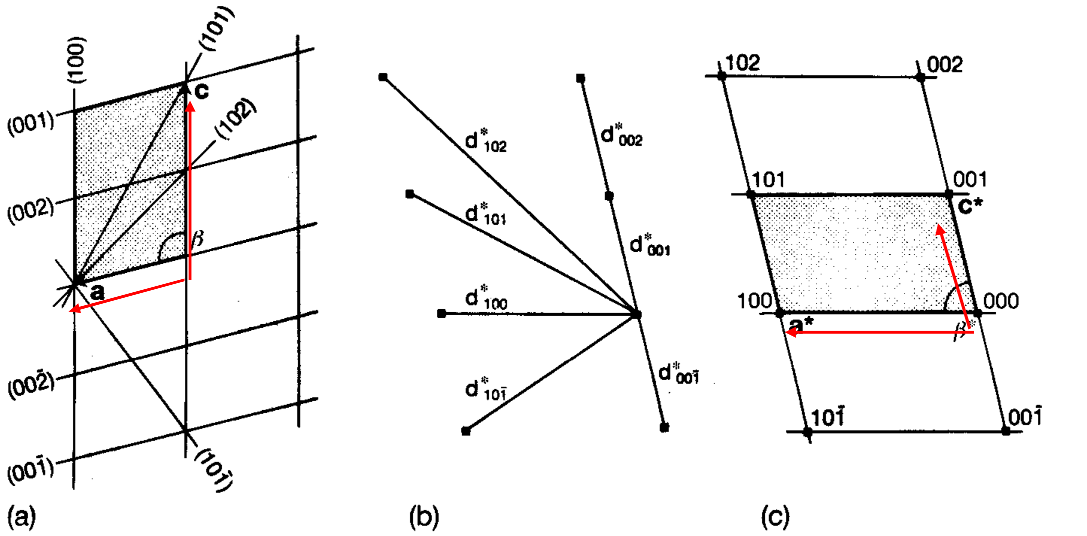


Fig 6.4 (a) Plan of a monoclinic *P* unit cell perpendicular to the *y*-axis with the unit cell shaded. The traces of some planes of type $\{h0l\}$ (i.e. parallel to the *y*-axis) are indicated, (b) the reciprocal (lattice) vectors, $\mathbf{d}^*_{hkl}$ for these planes and (c) the reciprocal lattice 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.

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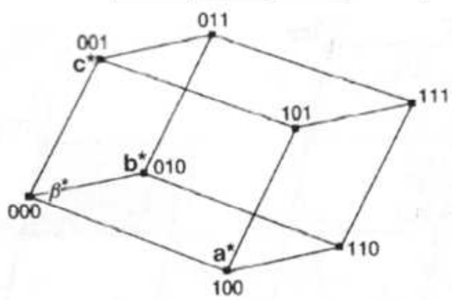
Reciprocal Lattice of a monoclinic P



Reciprocal lattice unit cell of a monoclinic P crystal

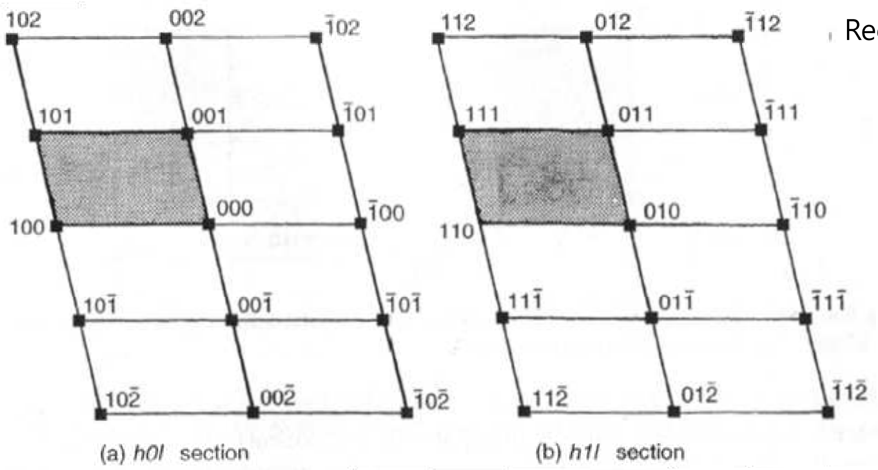


Fig. 6.5. Sections of a monoclinic reciprocal lattice perpendicular to the **b*** vector or y^*-axis. (a) $h0l$ section through the origin 000, built up by simply extending the section in Fig. 6.4(c); (b) $h1l$ section (representing planes intersecting the y-axis at one lattice vector **b**) 'one layer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

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Reciprocal Lattice

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

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

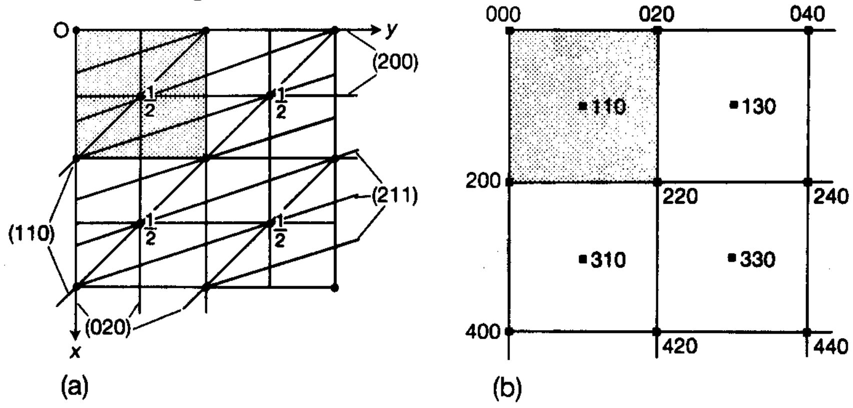
- Laue indices are simply the components of a reciprocal lattice vector

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

Laue indices, see page 141 of Hammond

Reciprocal lattice of a cubic - I

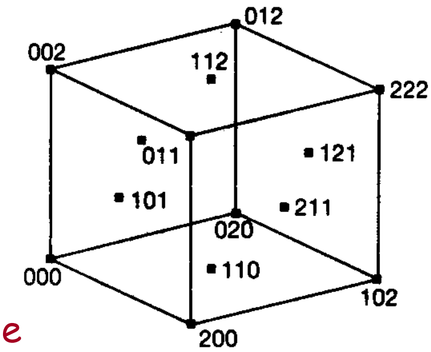
Fig. 6.4. (a) Plan of a cubic *I* crystal perpendicular to the *z*-axis and (b) pattern of reciprocal lattice points perpendicular to the *z*-axis. Note the cubic *F* arrangement of reciprocal lattice points in this plane.



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

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

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



Cubic I direct lattice - Cubic F reciprocal lattice

Cubic F direct lattice - Cubic I reciprocal lattice

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Real vs reciprocal in Cubic

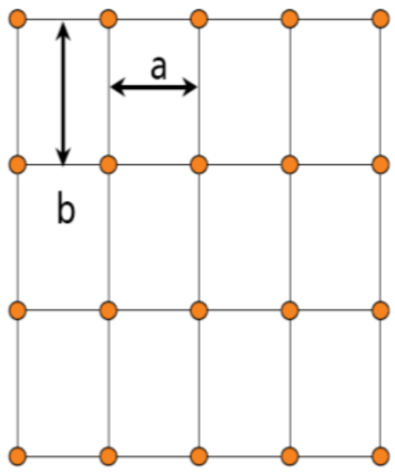
Real space	Reciprocal space
Cubic F (rhombohedral 60°)	Cubic I (rhombohedral 109.47°)
Cubic P (rhombohedral 90°)	Cubic P (rhombohedral 90°)
Cubic I (rhombehodral 109.47°)	Cubic F (rhombohedral 60°)

Real lattice ⟷ Fourier transform ⟷ Reciprocal lattice

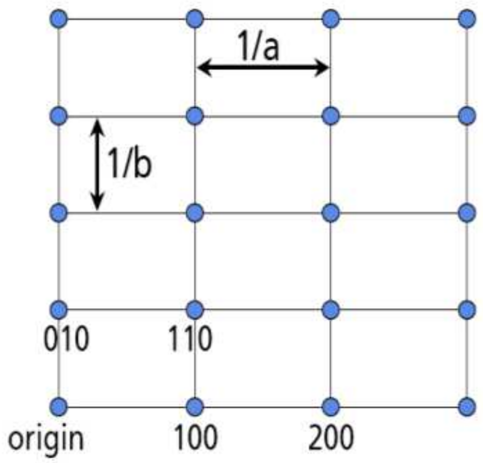
See Hammond Fig. 3.2

Reciprocal lattice

Real space



Reciprocal space



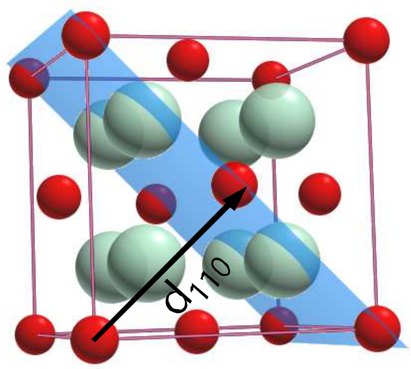
Points → atomic positions

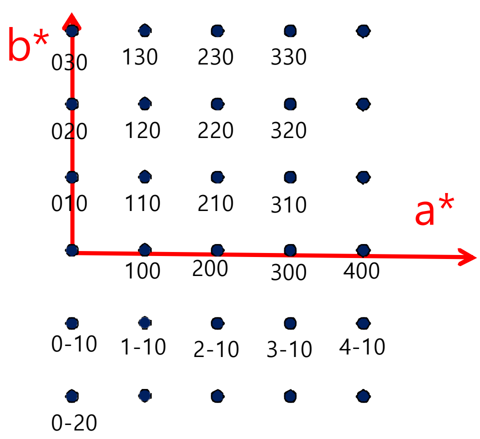
Points → (hkl), reflections

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 $d^*_{hkl} = 1/d_{hkl}$
- 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:

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

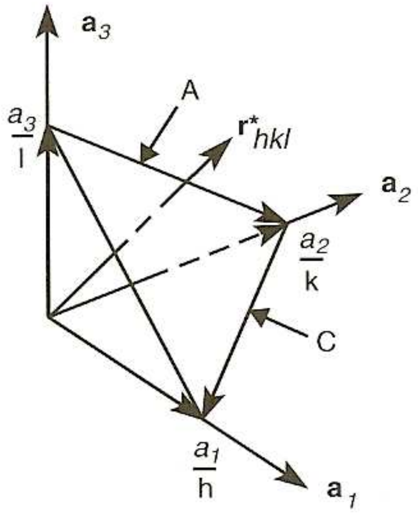




Scott A Speakman

Reciprocal lattice vector r*$_{hkl}$ is normal to real lattice plane (*hkl*)

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



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

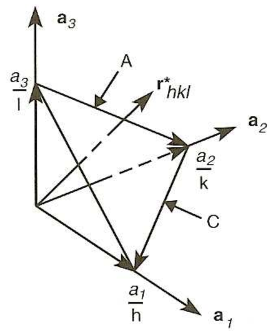
and

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

Thus

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

→ **A ⊥ r*$_{hkl}$ & C ⊥ *$_{hkl}$ → r*$_{hkl}$ ⊥ (*hkl*)**



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

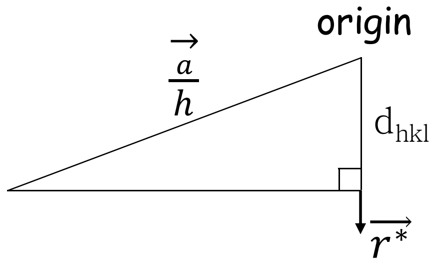
The magnitude of $\mathbf{r}^*_{hkl}$ *is the inverse of the interplanar spacing of the* (hkl) *planes,* d_{hkl}. The unit normal to (hkl) is given by $\mathbf{n} = \mathbf{r}^*_{hkl}/|\mathbf{r}^*_{hkl}|$ so that $\mathbf{n} = (h\mathbf{b}_1 + k\mathbf{b}_2 + l\mathbf{b}_3)/|\mathbf{r}^*_{hkl}|$. Referring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

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

Reciprocal lattice and interplanar spacing d_{hkl}



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

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

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

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

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

Interplanar spacing

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

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

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:

$$\frac{1}{d_{hkl}^2} = \frac{a_1^2a_2^2a_3^2}{V^2}\left[\frac{h^2\sin^2\alpha}{a_1^2} + \frac{k^2\sin^2\beta}{a_2^2} + \frac{l^2\sin^2\gamma}{a_3^2} + \frac{2hk}{a_1a_2}(\cos\alpha\cos\beta - \cos\gamma) + \frac{2kl}{a_2a_3}(\cos\beta\cos\gamma - \cos\alpha) + \frac{2lh}{a_1a_3}(\cos\gamma\cos\alpha - \cos\beta)\right] \quad (2.9)$$

Interplanar spacing d_{hkl}

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

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

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

Rhombohedral:

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

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

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

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),

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

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

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

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

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

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

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

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

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