Chapter 2 Lattice and Its Properties

Reading Assignment:

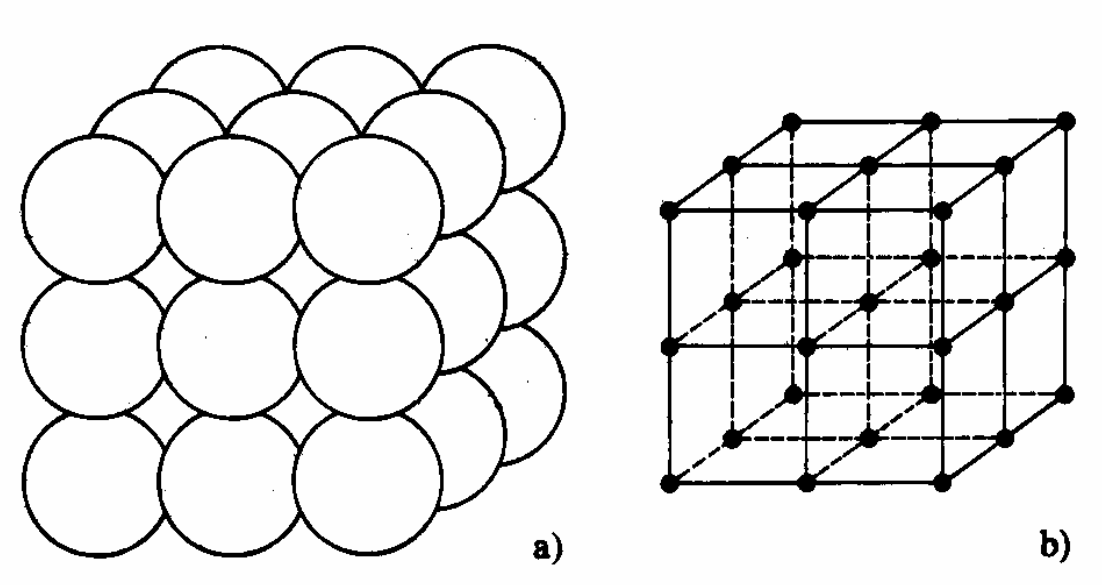
1. W. B-Ott, Crystallography-chapter 2

Contents

Lattice (격자)

Crystal- three-dimensional periodic arrangement of atoms, ions, or molecules- translational periodicity (병진주기)

ex) α-polonium

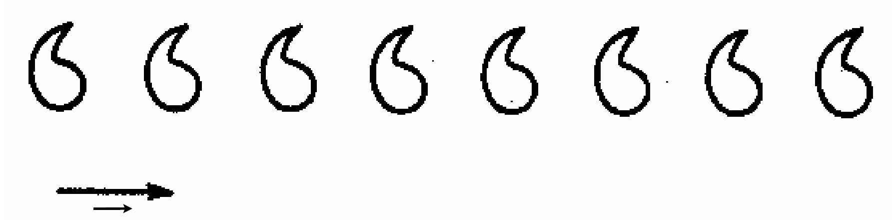


each atom- its center of gravity- point or space lattice

- pure mathematical concept

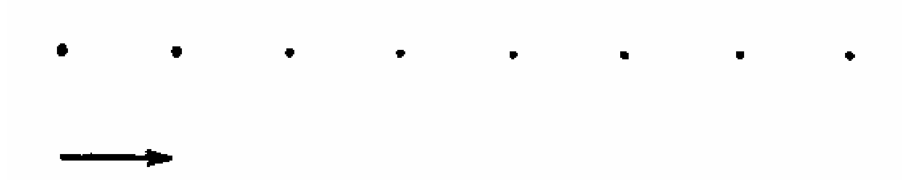
Translation (병진)

Pattern produced by periodic repetition in one dimension and defined by translation , $\vec{a}$



$\vec{a}$

motif- point identical (or equivalent) point (동가점)



$\vec{a}$

Line lattice (선격자) $|\vec{a}| = a$: lattice parameter (constant)

For any translation in 1-D

$$T = m\vec{a} \qquad -\infty < m < \infty$$

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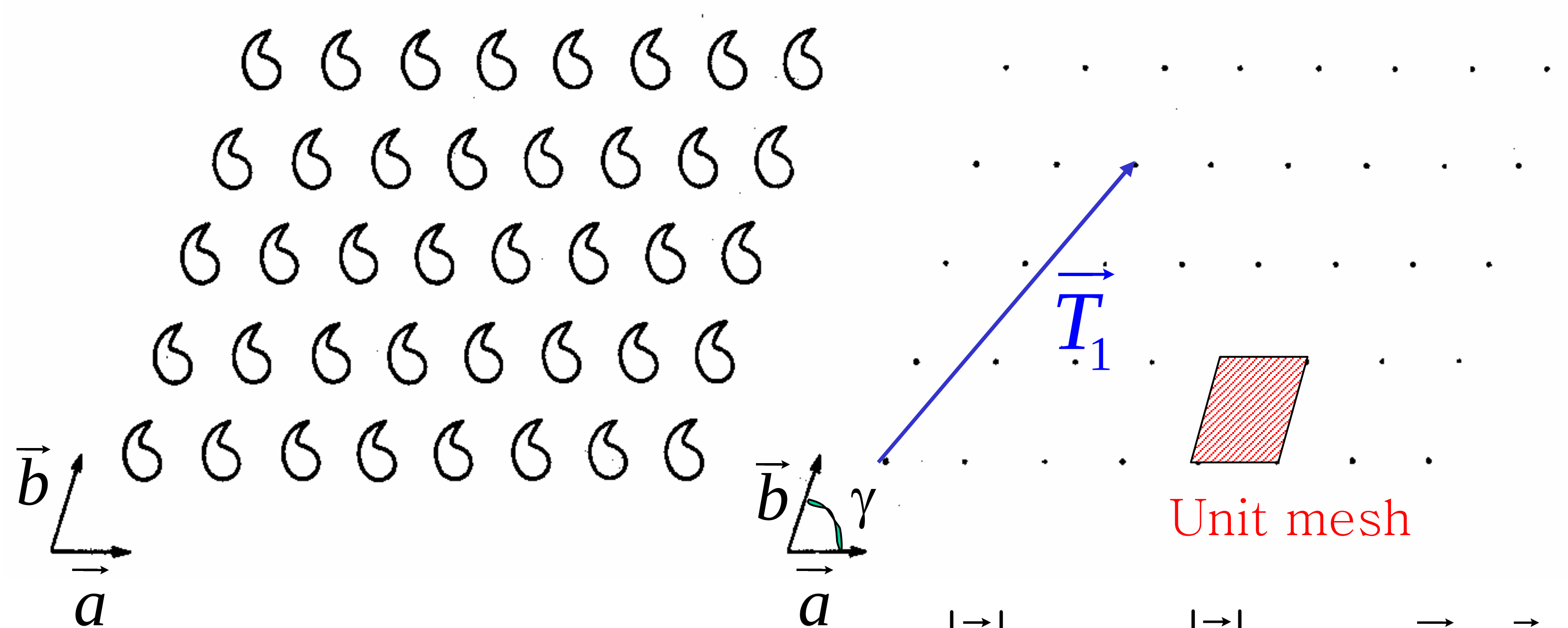
Pattern produced by periodic repetition in two dimensional and defined by translation , $\vec{a}$ and $\vec{b}$



Plane lattice (면격자)

$$\left|\vec{a}\right| = a \qquad \left|\vec{b}\right| = b \qquad \vec{a} \wedge \vec{b} = \gamma$$

For any translation in 2-D

$$\vec{T} = m\vec{a} + n\vec{b} \qquad -\infty < m < \infty, -\infty < n < \infty$$

Ex) $\vec{T}_1 = 2\vec{a} + 3\vec{b}$

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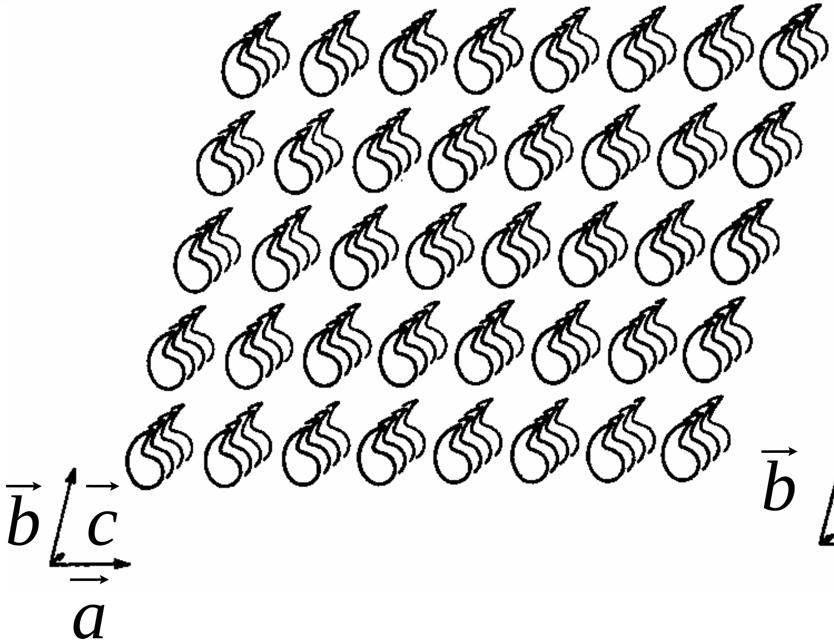
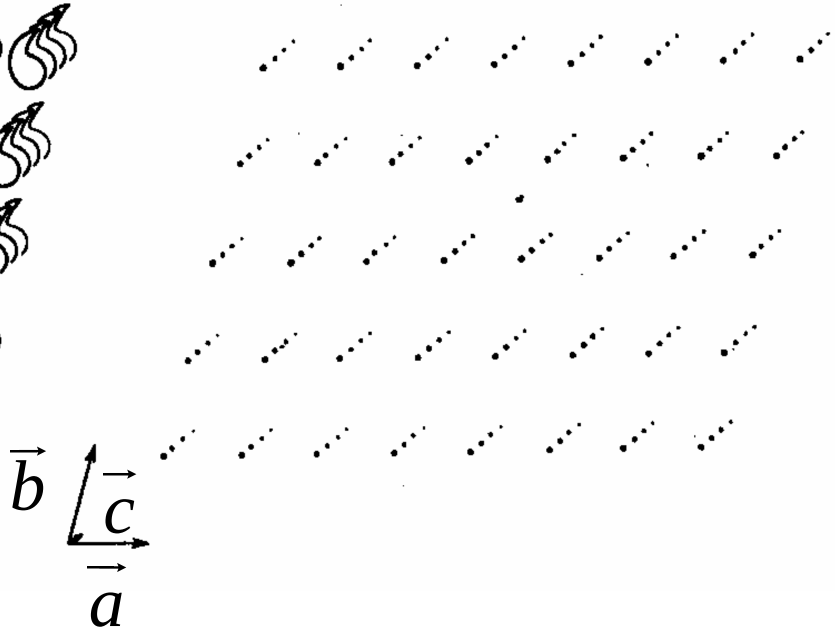
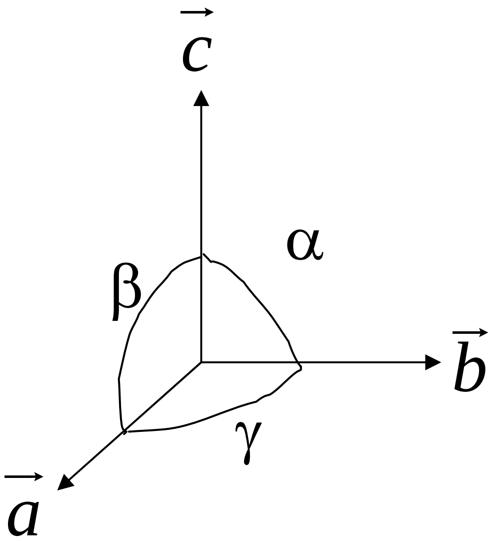
Space Lattice (공간격자)







Lattice constants

$$\left|\vec{a}\right| = a \qquad \vec{a} \wedge \vec{b} = \gamma$$

$$\left|\vec{b}\right| = b \qquad \vec{b} \wedge \vec{c} = \alpha$$

$$\left|\vec{c}\right| = c \qquad \vec{c} \wedge \vec{a} = \beta$$

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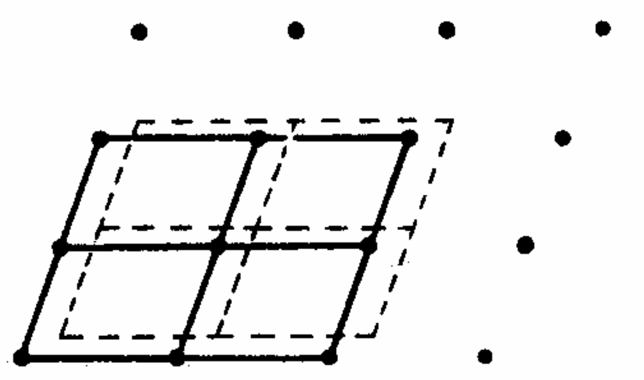
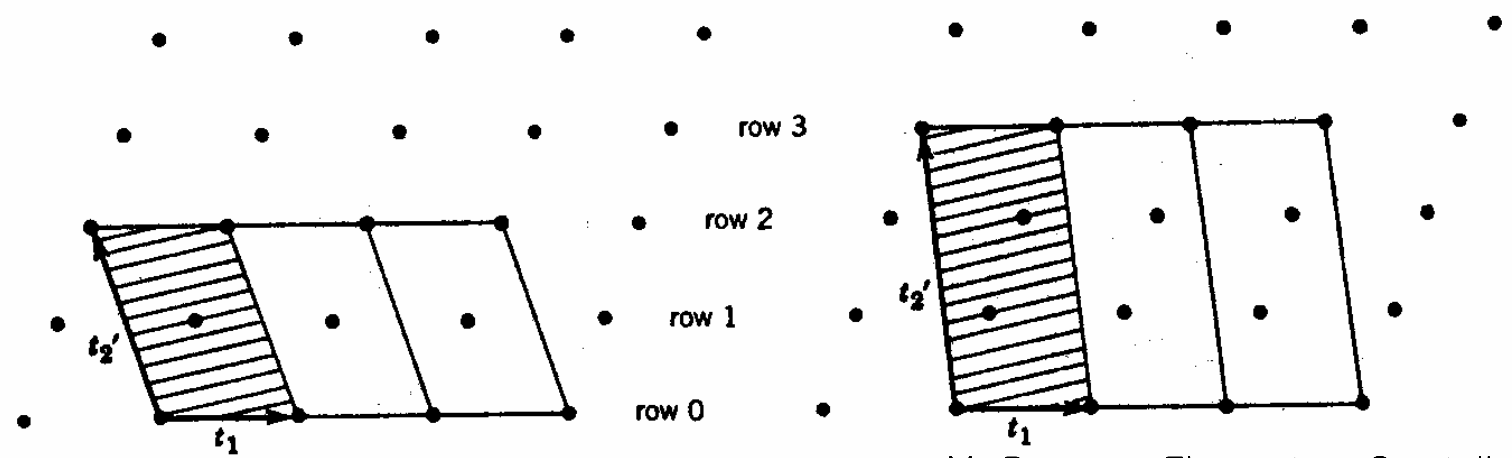
Lattice

For any translation

$$\vec{T} = m\vec{a} + n\vec{b} + p\vec{c} \qquad -\infty < m < \infty, -\infty < n < \infty, -\infty < p < \infty$$

- Primitive cell: one lattice point per cell
  Non-primitive cell
  Unit cell (C, I, F)





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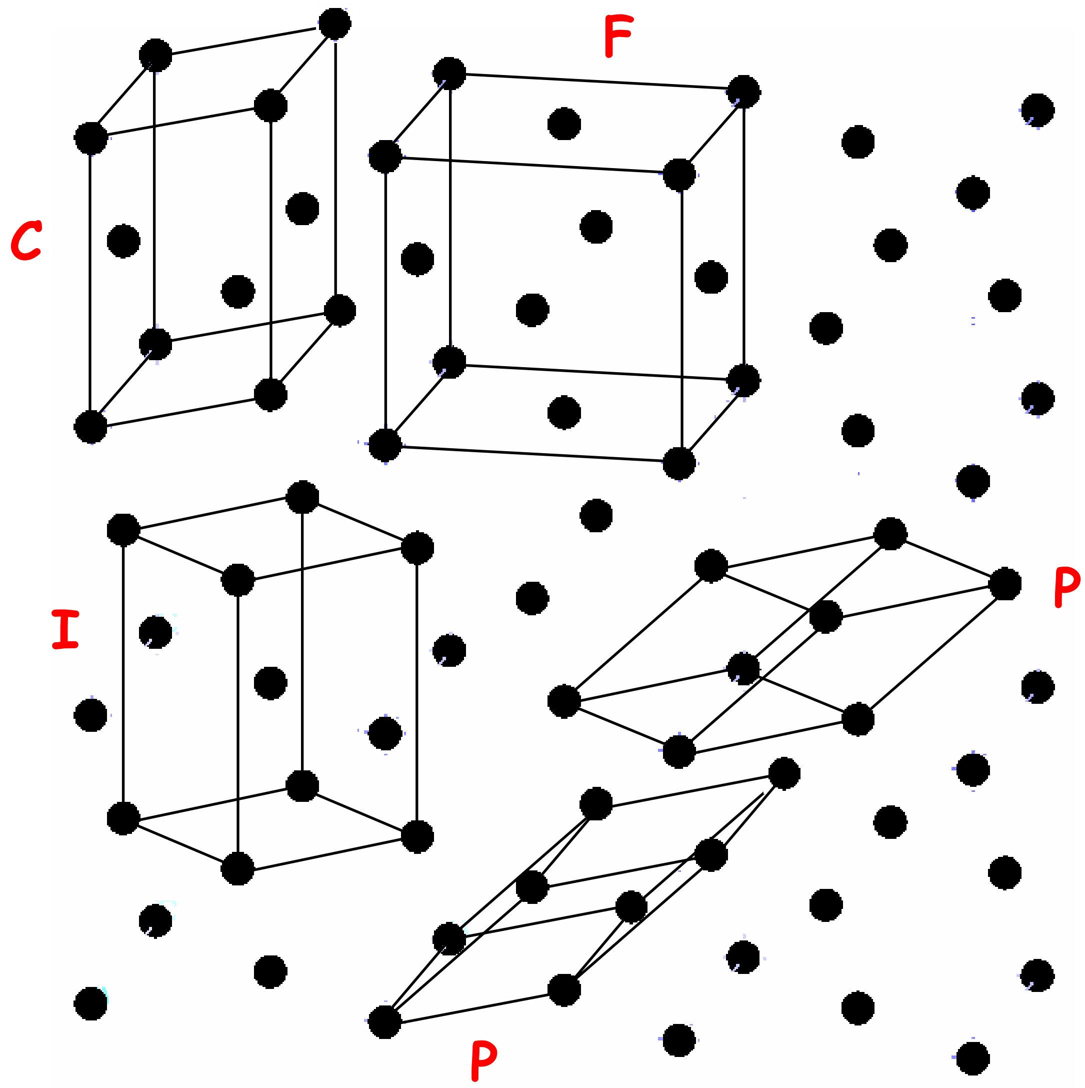
Lattice

➢ P, I, F, C

- ❑ *P* : **Primitive**
- ❑ *I* : **Body centered**
- ❑ *F* : **Face centered**
- ❑ *C* : **Base centered**



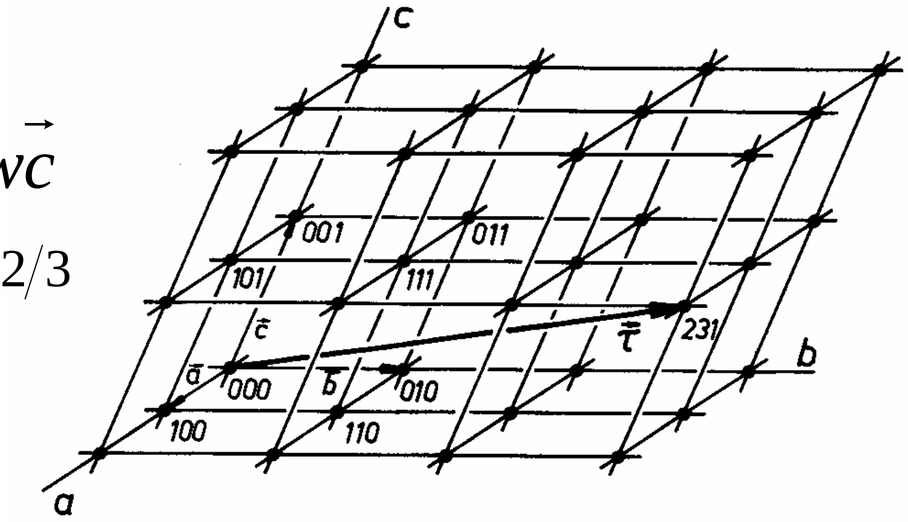
Lattice Point, Lattice Line

- Lattice point, uvw

$$\vec{T} = m\vec{a} + n\vec{b} + p\vec{c} = u\vec{a} + v\vec{b} + w\vec{c}$$

point- uvw, integer and 1/2 1/3 2/3

$\bar{u}\bar{v}\bar{w}$



- lattice line, [uvw]

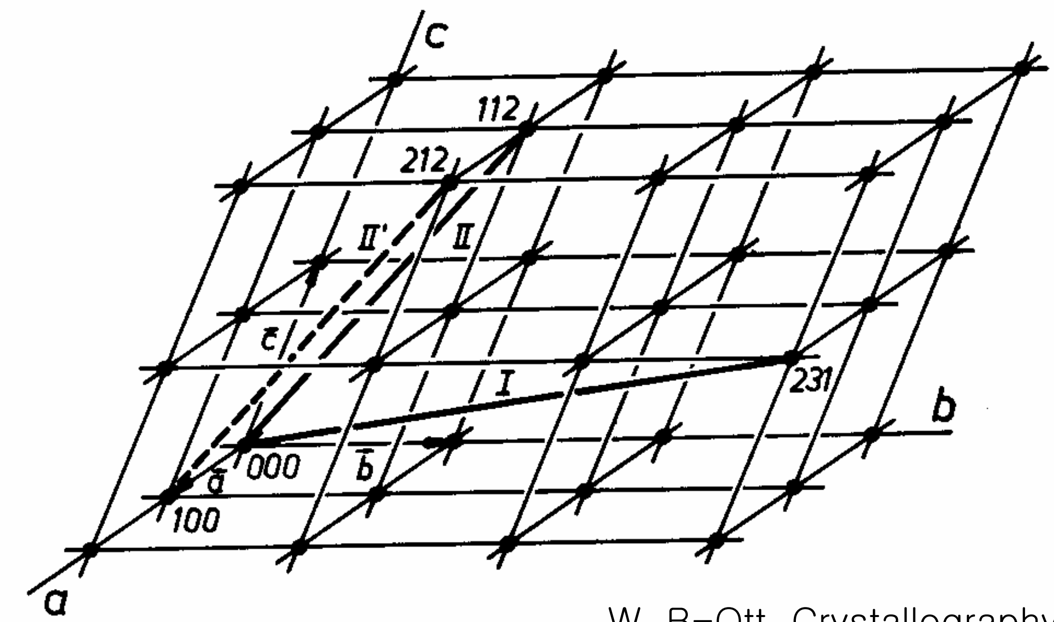
line- two points

I: 000 231 → [231]

II: 000 112 → [112]

II': 100 212 → [112]

family <uvw>



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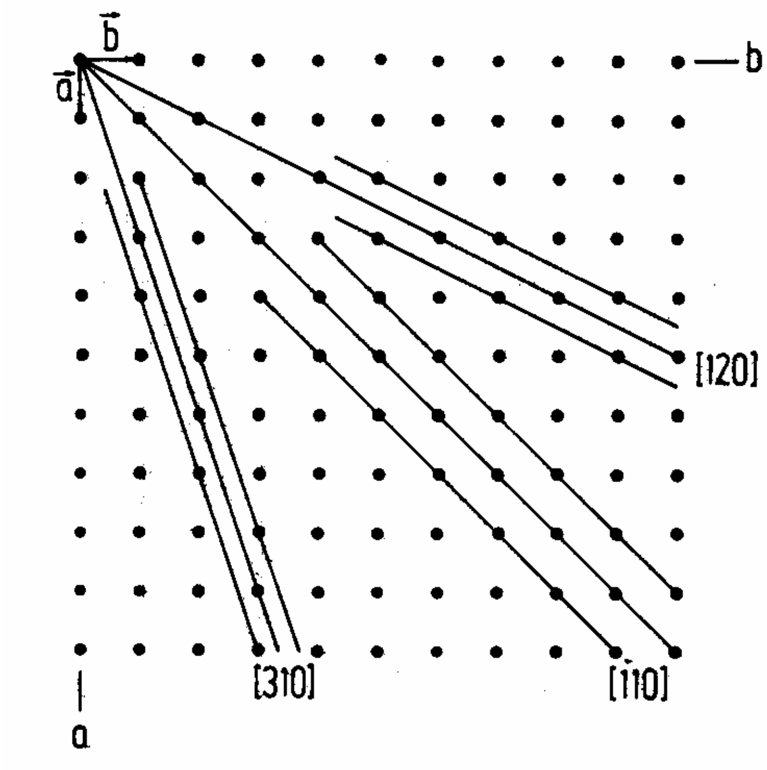
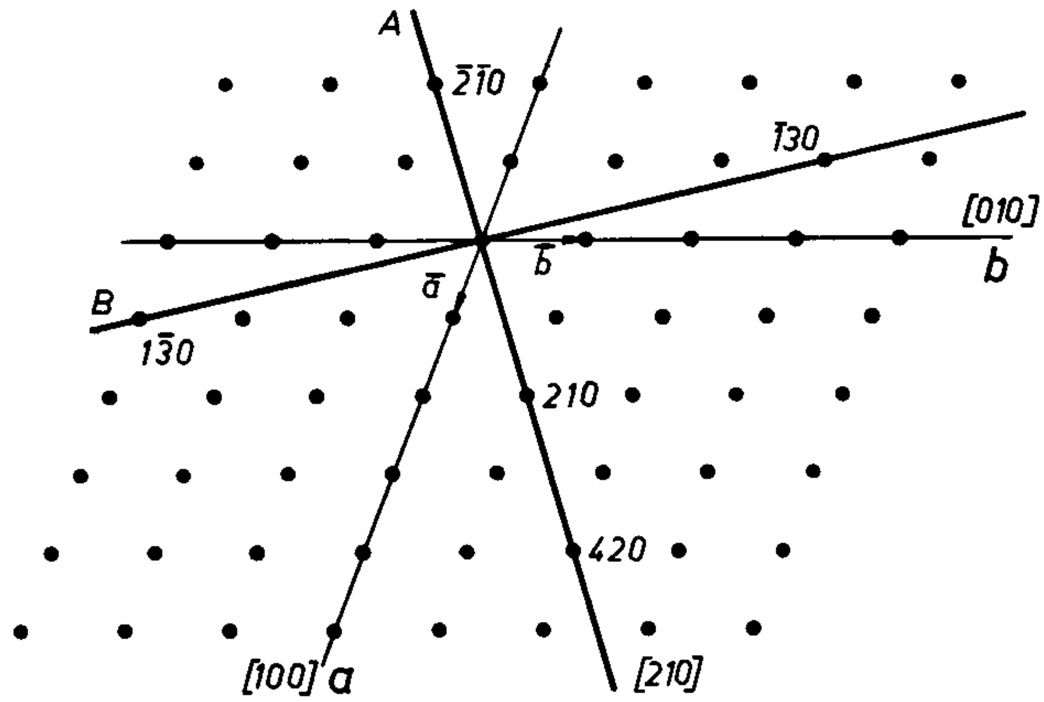
Lattice Line

* Note that the triple [uvw] describe not only a lattice line through the origin and the point uvw, but the infinite set of lattice lines which are parallel to it and have the same lattice parameter.





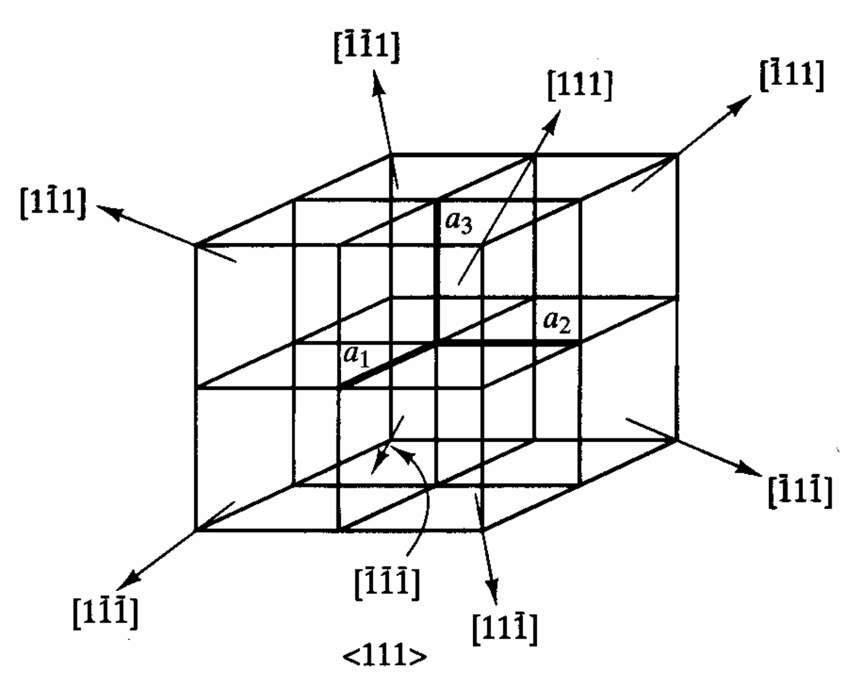
** smallest integer 210, 420, $\bar{2}\bar{1}\bar{0}$ → [210]

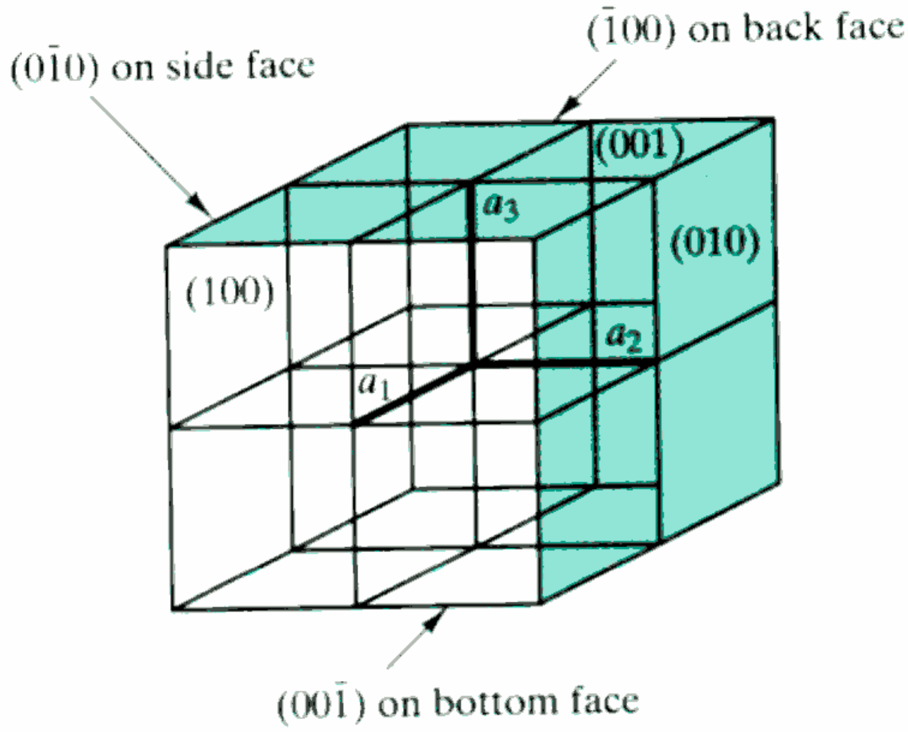
opposite direction $\bar{1}30$ and $1\bar{3}0$

A Family of Directions and Planes

- <111> angular bracket

- {100} braces

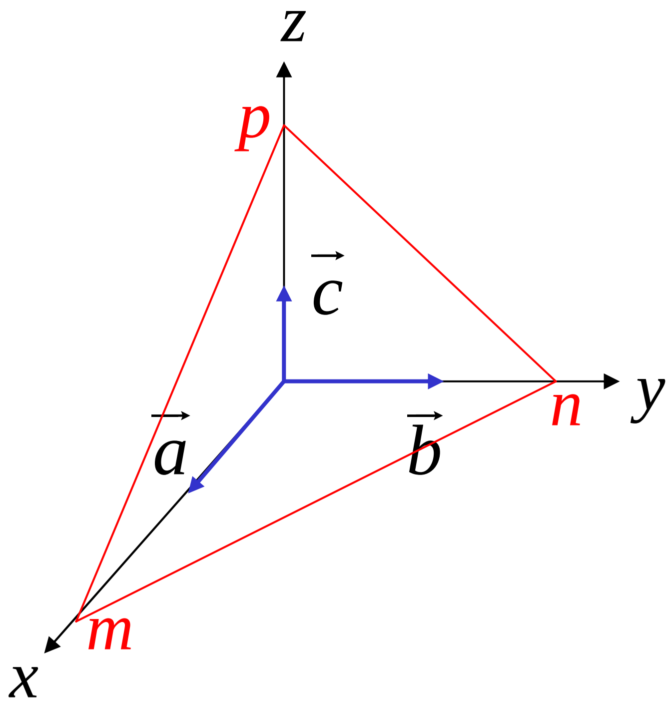




∗[111] square bracket

∗(100) parentheses

Lattice plane (Miller indices)



m00, 0n0, 00p: define lattice plane

m, n, ∞ : no intercepts with axes

reciprocal

$$h \sim \frac{1}{m} \qquad k \sim \frac{1}{n} \qquad l \sim \frac{1}{p}$$

smallest integer (hkl)

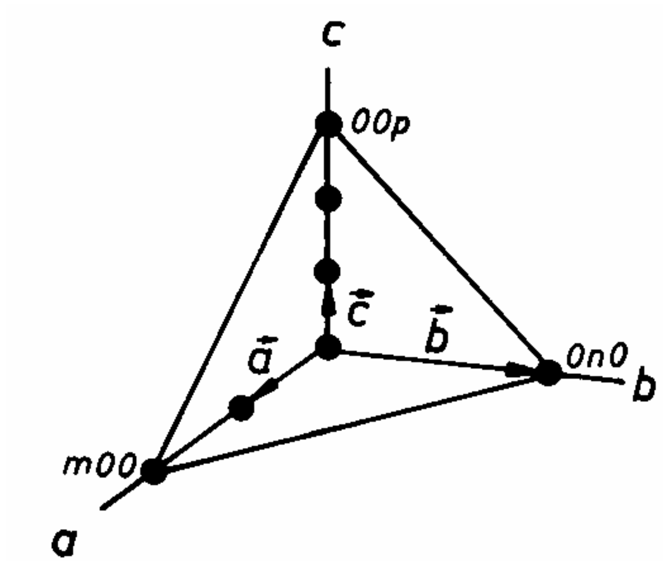
family {hkl}

2, 1, 3

1/2, 1/1, 1/3

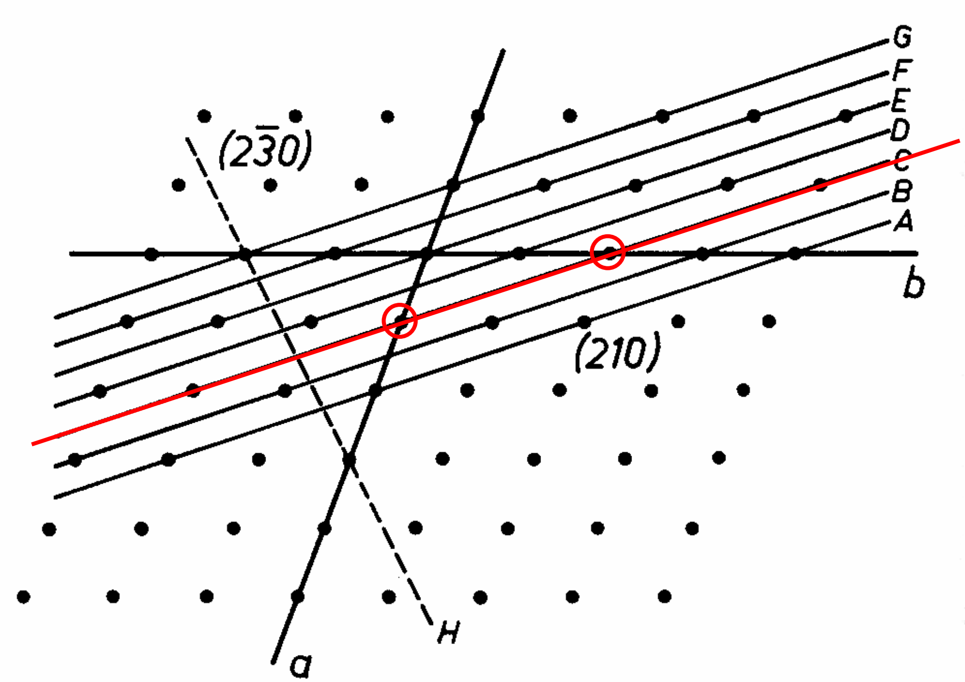
3, 6, 2

(362)



Lattice plane (Miller indices)

* The triple (hkl), which represents not merely a single plane, but an infinite set of parallel planes.



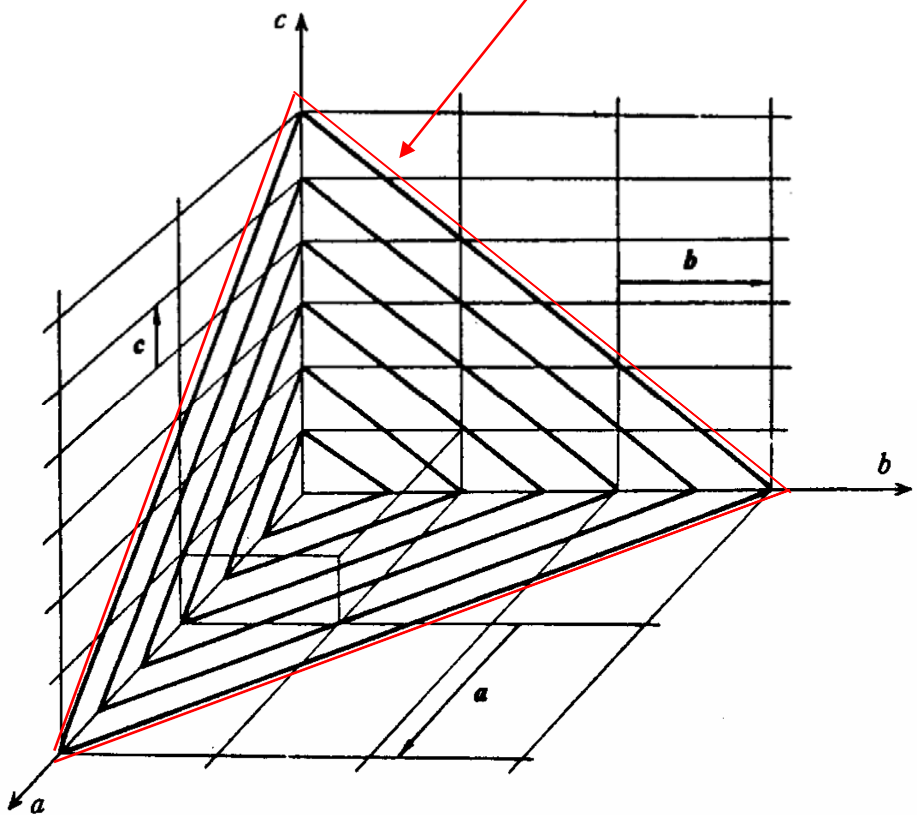
	m	n	p	$\frac{1}{m}$	$\frac{1}{n}$	$\frac{1}{p}$	(hkl)
A	2	4	∞	$\frac{1}{2}$	$\frac{1}{4}$	0	(210)
B	$\frac{3}{2}$	3	∞	$\frac{2}{3}$	$\frac{1}{3}$	0	(210)
C	1	2	∞	1	$\frac{1}{2}$	0	(210)
D	$\frac{1}{2}$	1	∞	2	1	0	(210)
E	–	–	–	–	–	–	
F	$\frac{\bar{1}}{2}$	$\bar{1}$	∞	$\bar{2}$	$\bar{1}$	0	($\bar{2}\bar{1}$0)
G	$\bar{1}$	$\bar{2}$	∞	$\bar{1}$	$\frac{\bar{1}}{2}$	0	($\bar{2}\bar{1}$0)
H	3	$\bar{2}$	∞	$\frac{1}{3}$	$\frac{\bar{1}}{2}$	0	(2$\bar{3}$0)

* As the indices rise, the spacing between the planes decreases, as does the density of points on each plane.

Lattice plane (Miller indices)

* There are *mnp/rst* equally spaced, identical planes from the origin to the rational intercept plane, where *r* is the highest common factor (HCF) of *m* and *n*, *s* the HCF of *n* and *p*, and *t* the HCF of *p* and *m*.

* rational intercept plane (유리교차면): 세 축상에서 모두 격자점과 교차하는 면



intercept	2,	3,	6
reciprocal	1/2,	1/3,	1/6
	3	2	1
		(321)	

r=1, s=3, t=2

mnp/rst= 2x3x6/1x3x2=6

6 planes between origin and rational intercept plane

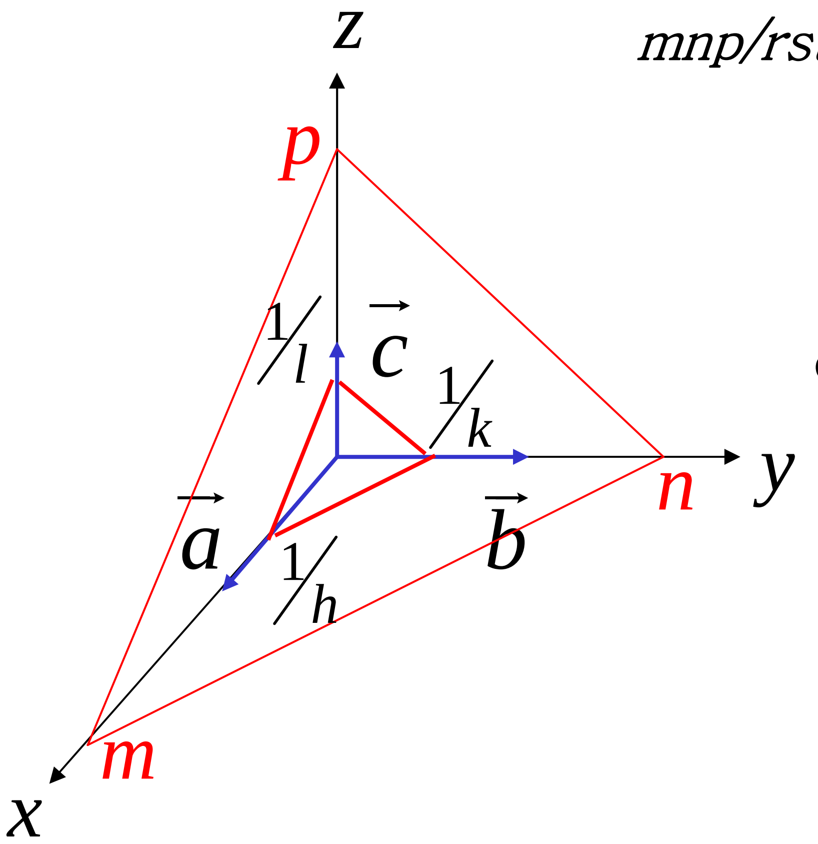
np/rst=3, pm/rst=2,mn/rst=1

|| || ||

h k l

Lattice plane (Miller indices)

Equation of a rational intercept plane $\frac{x}{m}+\frac{y}{n}+\frac{z}{p}=1$



mnp/rst planes between origin and this plane

$$\frac{np}{rst}x+\frac{pm}{rst}y+\frac{mn}{rst}z=\frac{mnp}{rst}$$

equation of the plane nearest to origin

$$\frac{np}{rst}x+\frac{pm}{rst}y+\frac{mn}{rst}z=1$$

$$hx+ky+lz=1 \qquad \frac{x}{\frac{1}{h}}+\frac{y}{\frac{1}{k}}+\frac{z}{\frac{1}{l}}=1$$

(hkl) plane: 세 축의 단위벡터 $\vec{a},\vec{b},\vec{c}$ 를 h, k, l 로 나누는 점에서 세축과 교차하게 됨

Zonal Equation

* The plane (khl) which cuts the origin has the equation:

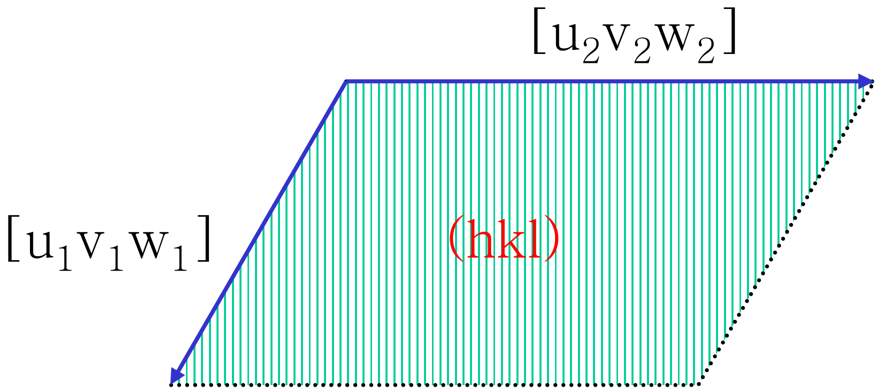
$$hx + ky + lz = 0$$

* A point u, v, w on the plane passing through the origin:

$$hu + kv + lw = 0$$ Zonal equation

* Two lattice lines $[u_1v_1w_1]$ and $[u_2v_2w_2]$ lie in the lattice plane (hkl) whose indices can be determined from the zonal equation:

$$hu_1 + kv_1 + lw_1 = 0 \qquad hu_2 + kv_2 + lw_2 = 0$$

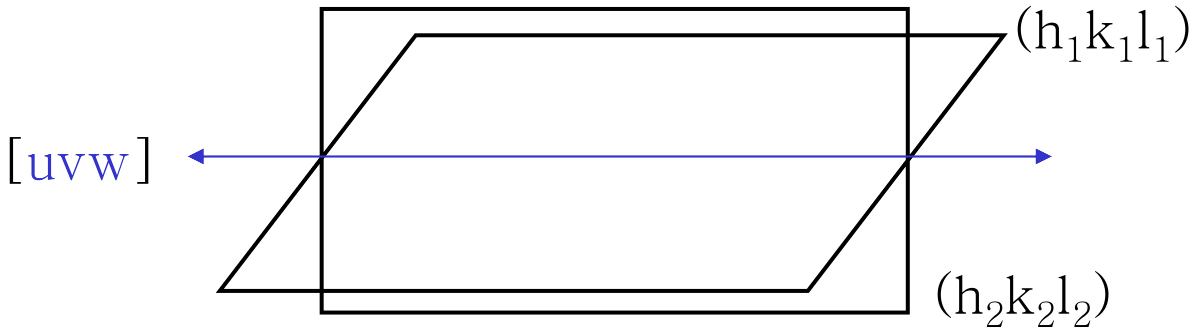


ex) $[10\bar{1}]$ and $[\bar{1}2\bar{1}]$

(111) plane

* The lattice planes $(h_1k_1l_1)$ and $(h_2k_2l_2)$ intersect in the lattice line [uvw] whose indices can be determined

$$h_1u + k_1v + l_1w = 0 \quad h_2u + k_2v + l_2w = 0$$

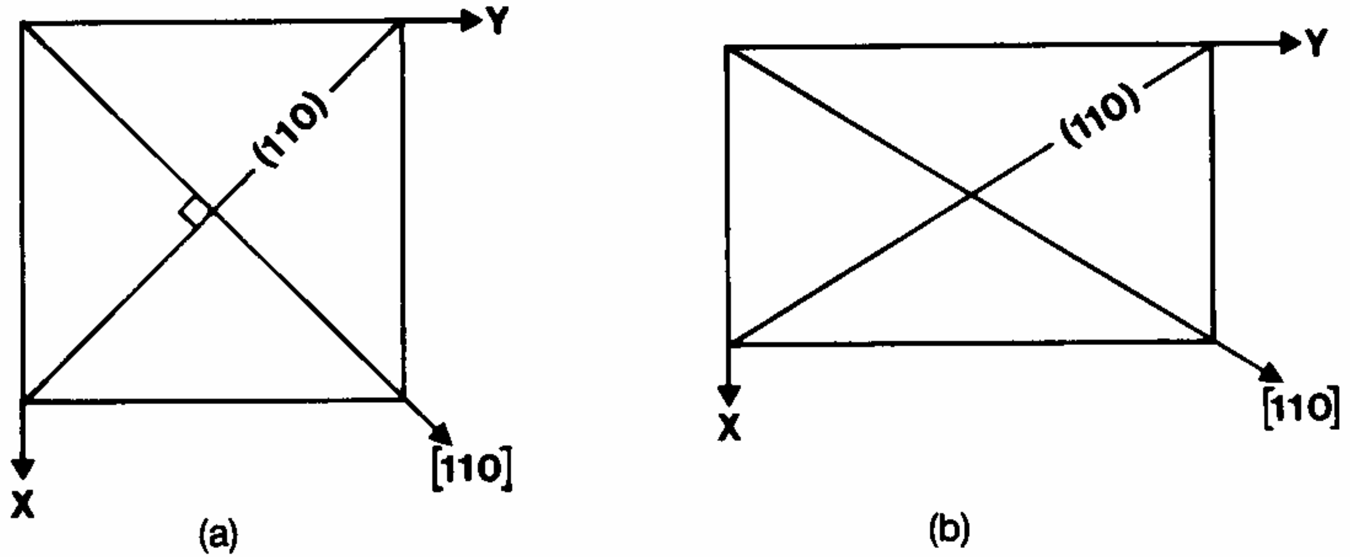


$$\begin{array}{c|ccccccccc|c}
h_1 & k_1 & & l_1 & & h_1 & & k_1 & l_1 \\
 & & \times^{-}_{+} & & \times^{-}_{+} & & \times^{-}_{+} & & \\
h_2 & k_2 & & l_2 & & h_2 & & k_2 & l_2 \\
\hline
 & & u & & v & & w & &
\end{array}$$

$$u = (k_1l_2 - k_2l_1); \quad v = (l_1h_2 - l_2h_1); \quad w = (h_1k_2 - k_2h_1).$$

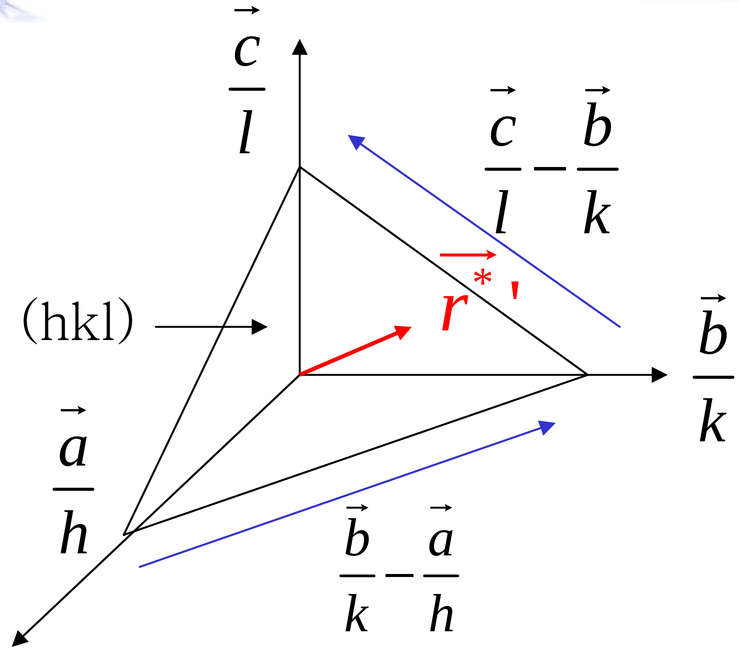
Direction vs. Planes of Same Indices

cubic orthorhombic



Plans of (a) cubic and (b) orthorhombic unit cells perpendicular to the z-axis, showing the relationships between planes and zone axes of the same numerical indices.

Reciprocal Lattice and Interplanar Spacing d_{hkl}



$$\overrightarrow{r^*}' = \left(\frac{\vec{b}}{k}-\frac{\vec{a}}{h}\right)\times\left(\frac{\vec{c}}{l}-\frac{\vec{b}}{k}\right)$$

$$= \frac{\vec{b}\times\vec{c}}{kl}+\frac{\vec{c}\times\vec{a}}{lh}+\frac{\vec{a}\times\vec{b}}{hk}$$

$$= \frac{abc}{hkl}\left(h\frac{\vec{b}\times\vec{c}}{abc}+k\frac{\vec{c}\times\vec{a}}{abc}+l\frac{\vec{a}\times\vec{b}}{abc}\right)$$

$$\overrightarrow{r^*} = h\frac{\vec{b}\times\vec{c}}{abc}+k\frac{\vec{c}\times\vec{a}}{abc}+l\frac{\vec{a}\times\vec{b}}{abc} = ha^*+kb^*+lc^* \qquad abc = \vec{a}\bullet\vec{b}\times\vec{c}$$

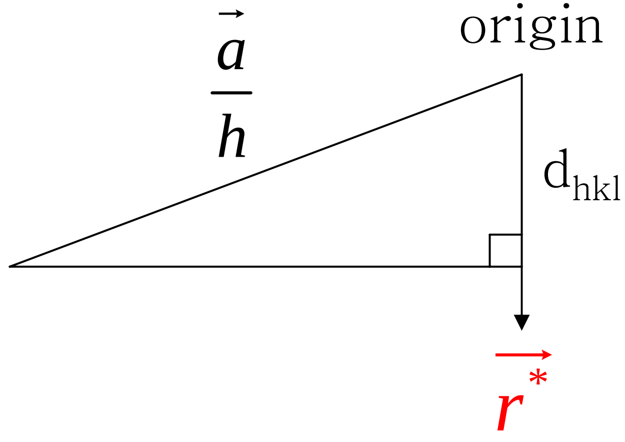
$$\overrightarrow{a^*} = \frac{\vec{b}\times\vec{c}}{abc} \qquad \overrightarrow{b^*} = \frac{\vec{c}\times\vec{a}}{abc} \qquad \overrightarrow{c^*} = \frac{\vec{a}\times\vec{b}}{abc}$$

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

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

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

Reciprocal lattice and interplanar spacing d_{hkl}



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

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

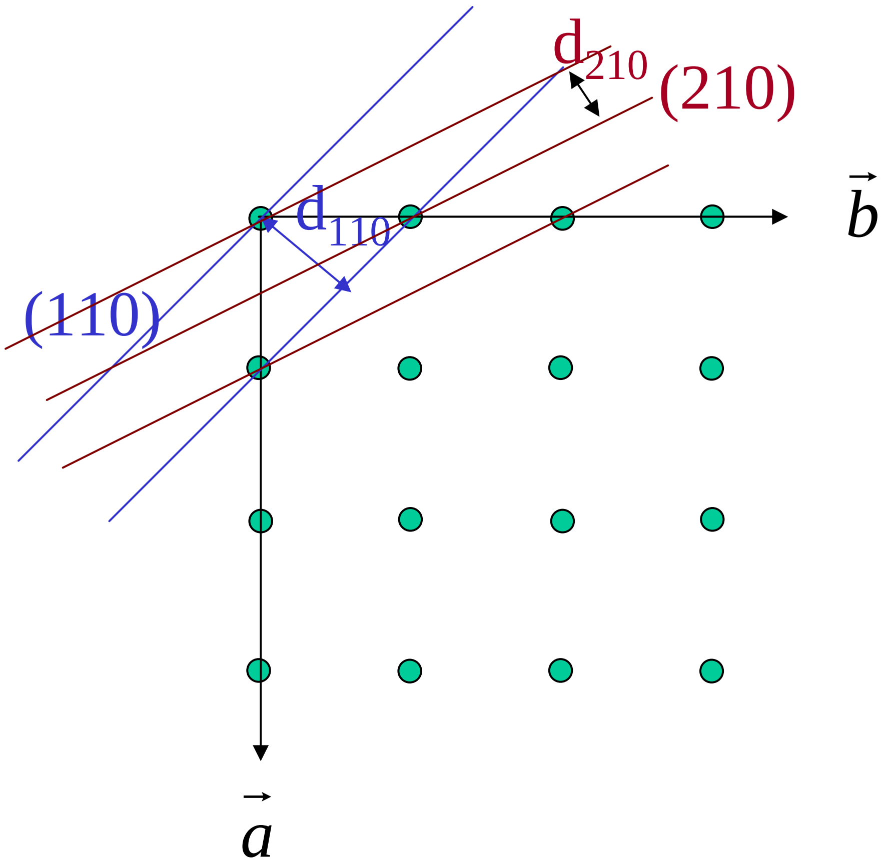
$$= h^2 a^{*2} + k^2 b^{*2} + l^2 c^{*2} + 2a^* b^* \cos\gamma^* + 2b^* c^* \cos\alpha^* + 2c^* a^* \cos\beta^*$$

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

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

Interplanar spacing d_{hkl}

For cubic



$$d_{110} = \frac{a}{\sqrt{1^2 + 1^2 + 0^2}} = \frac{a}{\sqrt{2}}$$

$$d_{210} = \frac{a}{\sqrt{2^2 + 1^2 + 0^2}} = \frac{a}{\sqrt{5}}$$

Angle between two planes

Calculating the angle between two planes

For cubic crystals, the angle, ϕ between two planes, $(h_1\ k_1\ l_1)$ and $(h_2\ k_2\ l_2)$ is given by:

$$\cos\phi = \frac{h_1h_2 + k_1k_2 + l_1l_2}{\sqrt{h_1^2 + k_1^2 + l_1^2}\sqrt{h_2^2 + k_2^2 + l_2^2}}$$

Example:

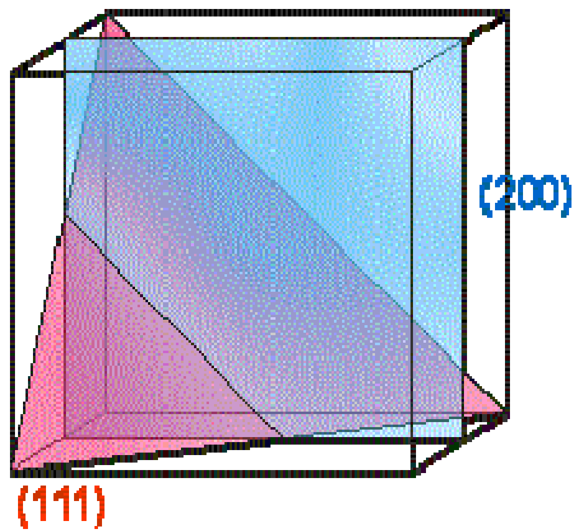
Calculate the angle between the (111) and (200) planes.

From the above,

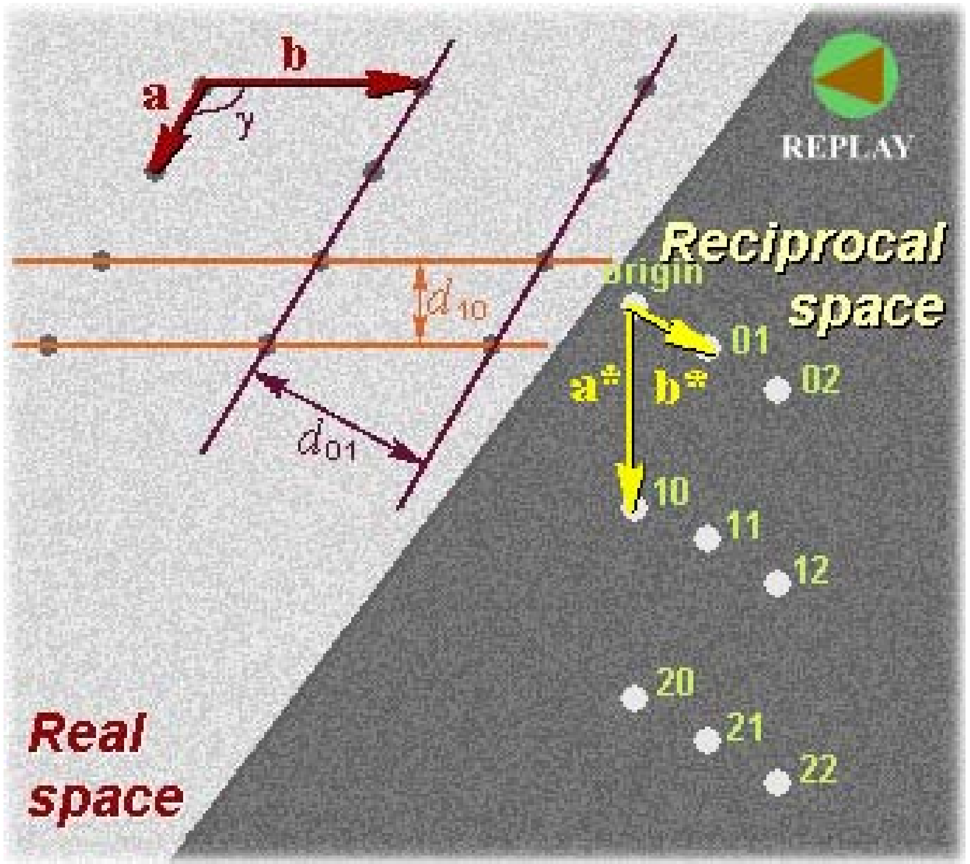
$$\cos\phi = \frac{(1\times 2) + (1\times 0) + (1\times 0)}{\sqrt{1+1+1}\sqrt{4+0+0}}$$

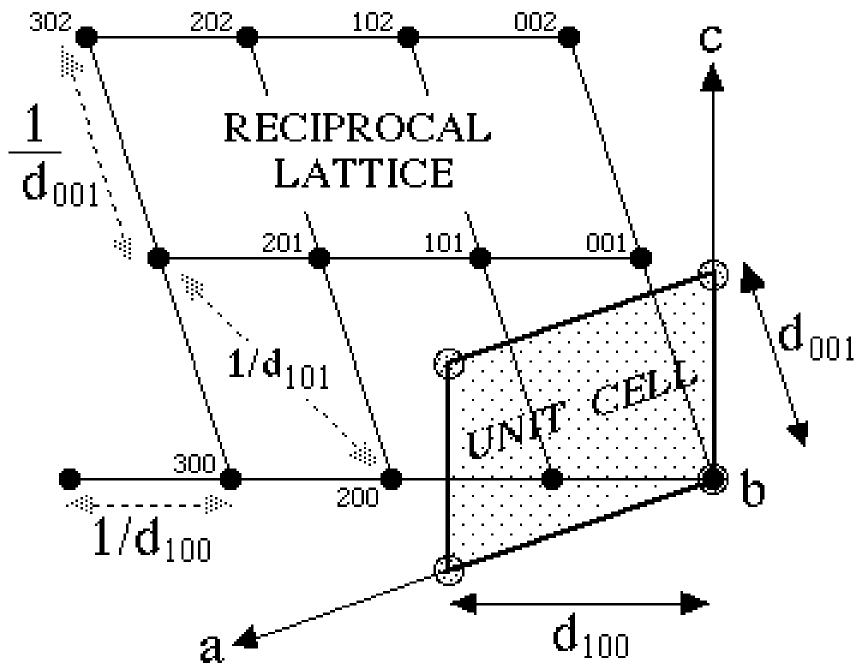
$$\cos\phi = \frac{1}{\sqrt{3}}$$

which produces the result, ϕ = 54.75?



Reciprocal lattice

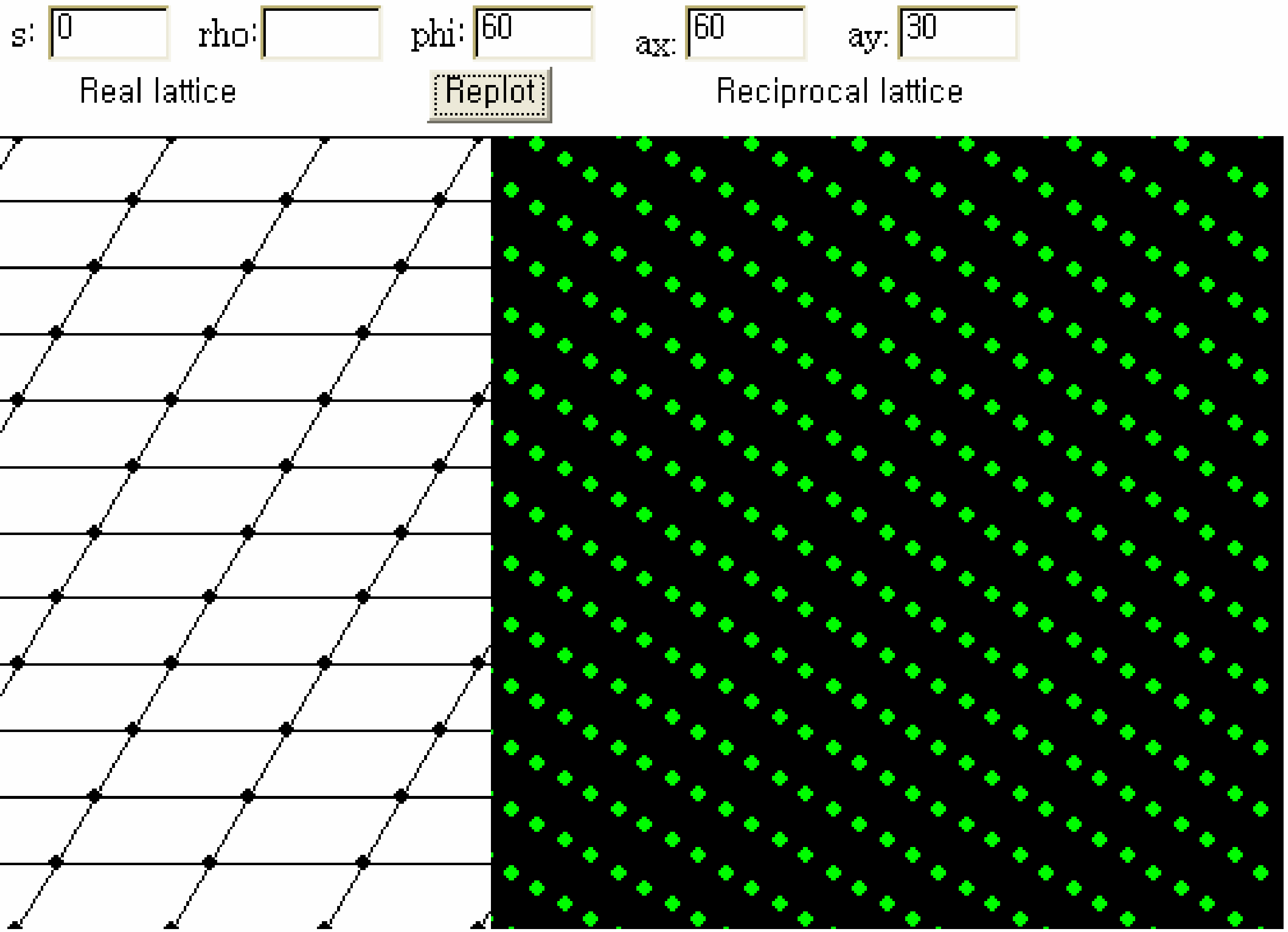




http://www.matter.org.uk/diffraction/geometry/2D_reciprocal_lattices.htm

http://www.humboldt.edu/~gdg1/recip.html

Reciprocal lattice



http://buckminster.physics.sunysb.edu/intlearn/lattice/lattice.html

Reciprocal Lattice

표 1.2 실격자와 역격자의 단위 수치간의 관계

$$a^* = \frac{bc \sin \alpha}{V} \qquad \cos \alpha^* = \frac{\cos \beta \cos \gamma - \cos \alpha}{\sin \beta \sin \gamma}$$

$$b^* = \frac{ca \sin \beta}{V} \qquad \cos \beta^* = \frac{\cos \gamma \cos \alpha - \cos \beta}{\sin \gamma \sin \alpha}$$

$$c^* = \frac{ab \sin \gamma}{V} \qquad \cos \gamma^* = \frac{\cos \alpha \cos \beta - \cos \gamma}{\sin \alpha \sin \beta}$$

$$a = \frac{b^* c^* \sin \alpha^*}{V^*} \qquad \cos \alpha = \frac{\cos \beta^* \cos \gamma^* - \cos \alpha^*}{\sin \beta^* \sin \gamma^*}$$

$$b = \frac{c^* a^* \sin \beta^*}{V^*} \qquad \cos \beta = \frac{\cos \gamma^* \cos \alpha^* - \cos \beta^*}{\sin \gamma^* \sin \alpha^*}$$

$$c = \frac{a^* b^* \sin \gamma^*}{V^*} \qquad \cos \gamma = \frac{\cos \alpha^* \cos \beta^* - \cos \gamma^*}{\sin \alpha^* \sin \beta^*}$$

$$V^* = a^* b^* c^* \sqrt{1 - \cos^2 \alpha^* - \cos^2 \beta^* - \cos^2 \gamma^* + 2 \cos \alpha^* \cos \beta^* \cos \gamma^*}$$

$$V = abc \sqrt{1 - \cos^2 \alpha - \cos^2 \beta - \cos^2 \gamma + 2 \cos \alpha \cos \beta \cos \gamma}$$

표 1.3 면간거리

	결정축계	$\frac{1}{d_{hkl}^2}$
cubic	입 방	$\frac{1}{a^2}(h^2+k^2+l^2)$
tetragonal	정 방	$\frac{h^2+k^2}{a^2}+\frac{l^2}{c^2}$
orthorhombic	사 방	$\frac{h^2}{a^2}+\frac{k^2}{b^2}+\frac{l^2}{c^2}$
hexagonal	육 방	$\frac{4}{3a^2}(h^2+hk+k^2)+\frac{l^2}{c^2}$
rhombohedral	능 면	$\frac{1}{a^2}\frac{(h^2+k^2+l^2)\sin^2\alpha+2(hk+kl+lh)(\cos^2\alpha-\cos\alpha)}{1+2\cos^2\alpha-3\cos^2\alpha}$
monoclinic	단 사	$\frac{\frac{h^2}{a^2}+\frac{k^2}{b^2}-\frac{2kh\cos\gamma}{ab}}{\sin^2\gamma}+\frac{l^2}{c^2}$ (first setting)
		$\frac{\frac{h^2}{a^2}+\frac{l^2}{c^2}-\frac{2hl\cos\beta}{ac}}{\sin^2\beta}+\frac{k^2}{b^2}$ (second setting)
triclinic	삼 사	$\frac{\frac{h^2}{a^2}\sin^2\alpha+\frac{k^2}{b^2}\sin^2\beta+\frac{l^2}{c^2}\sin^2\gamma+\frac{2hk}{ab}(\cos\alpha\cos\beta-\cos\gamma)+\frac{2kl}{bc}(\cos\beta\cos\gamma-\cos\alpha)+\frac{2lh}{ca}(\cos\gamma\cos\alpha-\cos\beta)}{1-\cos^2\alpha-\cos^2\beta-\cos^2\gamma+2\cos\alpha\cos\beta\cos\gamma}$

Reciprocal Lattice and Interplanar Spacing d_{hkl}

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

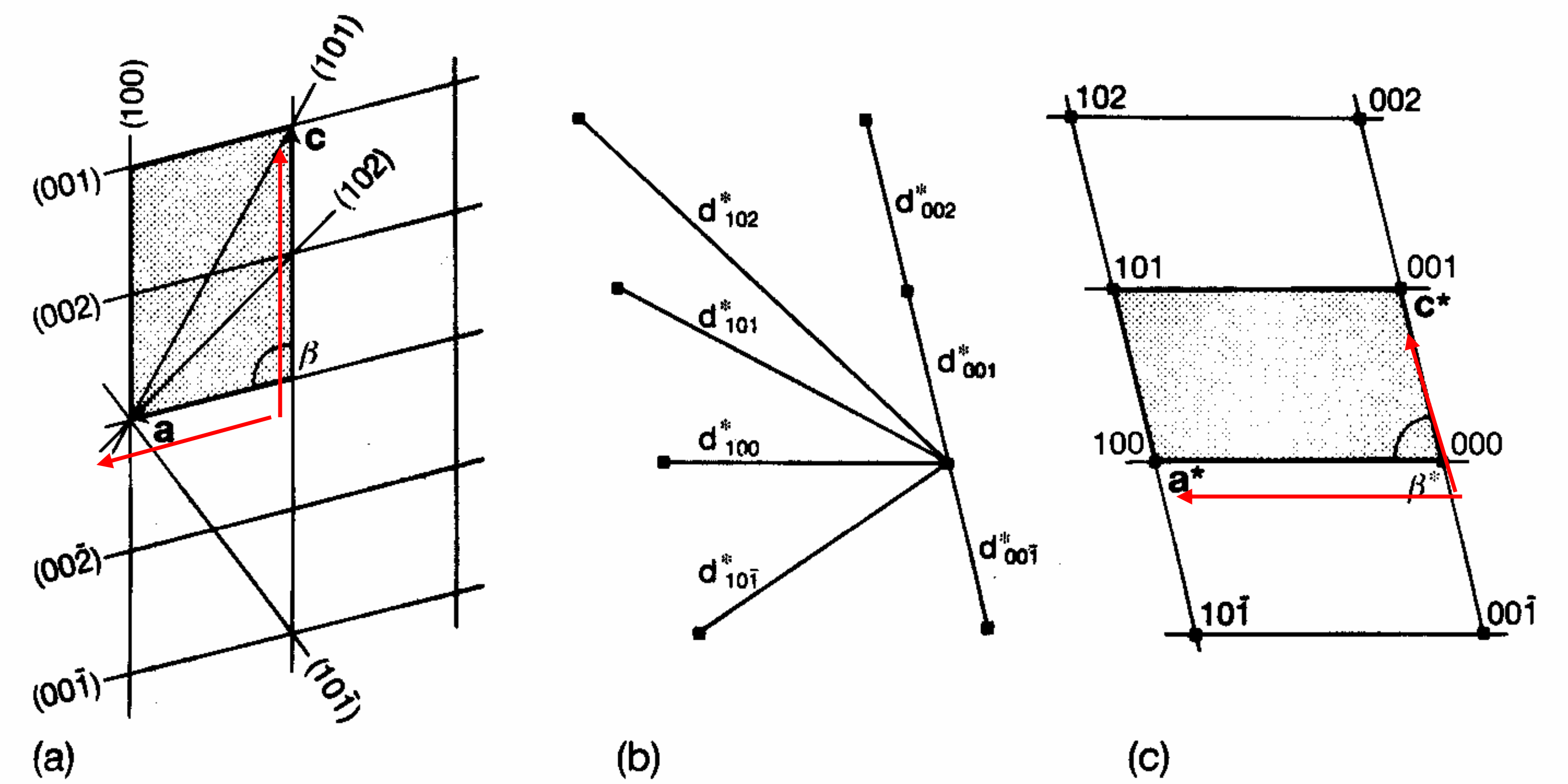


Fig. 6.2. (a) Plan of a monoclinic *P* unit cell perpendicular to the *y*-axis with the unit cell shaded. The traces of some planes of type $\{h0l\}$ (i.e. parallel to the *y*-axis) are indicated, (b) the reciprocal (lattice) vectors, $\mathbf{d}^*_{hkl}$ for these planes and (c) the reciprocal lattice 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.

Reciprocal lattice and interplanar spacing d_{hkl}

- cubic I $\quad a = b = c$

$$\alpha = \beta = \gamma = 90^o$$

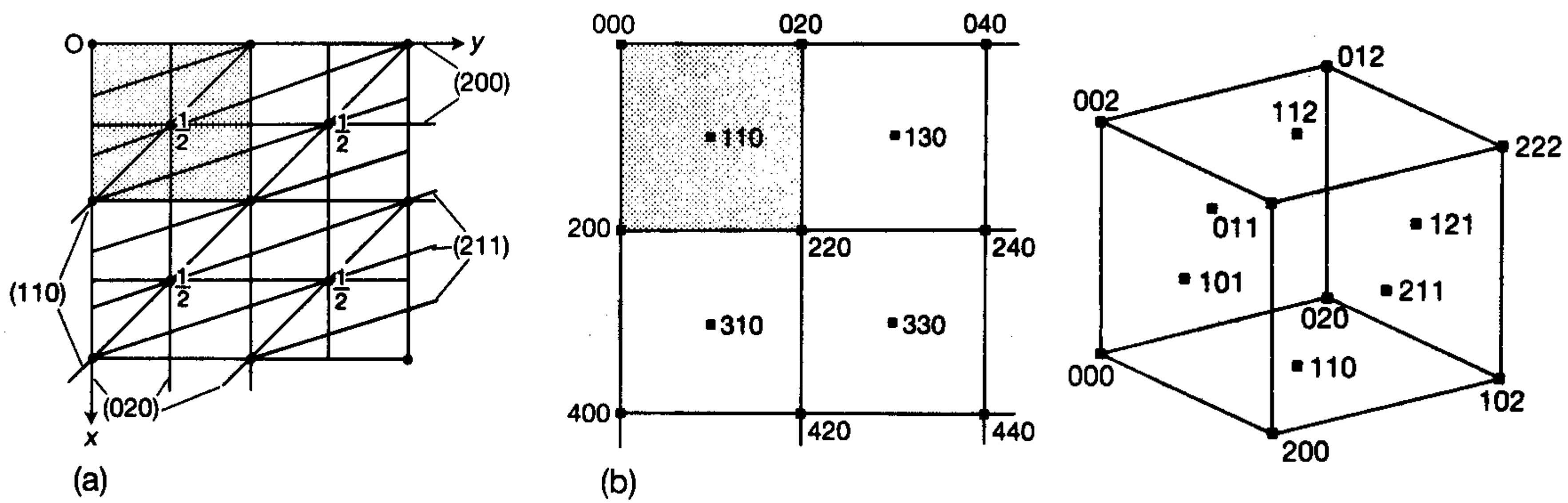
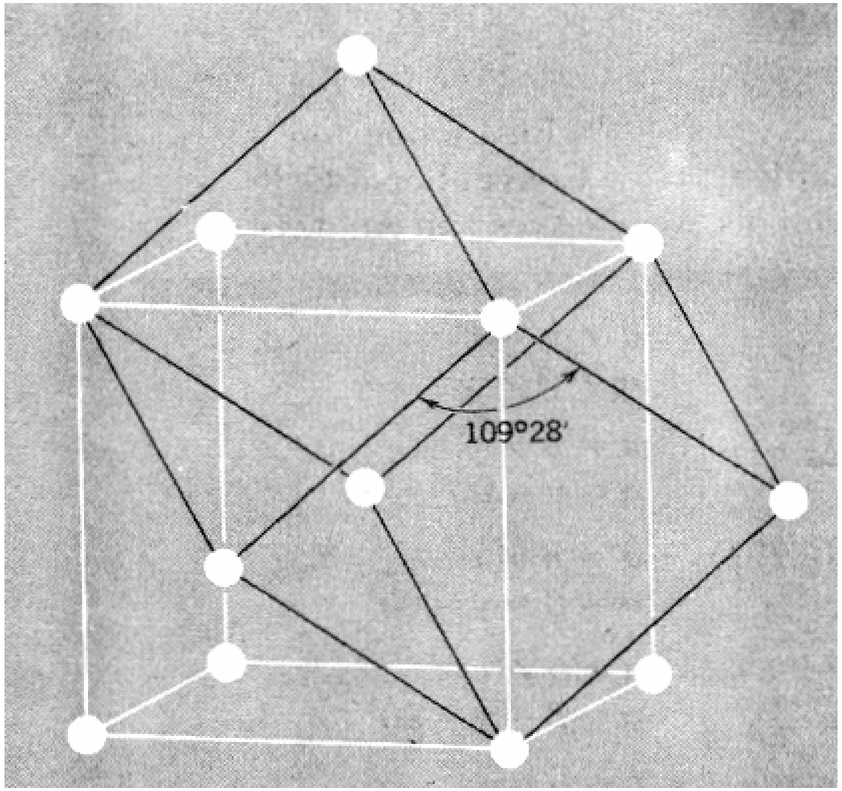
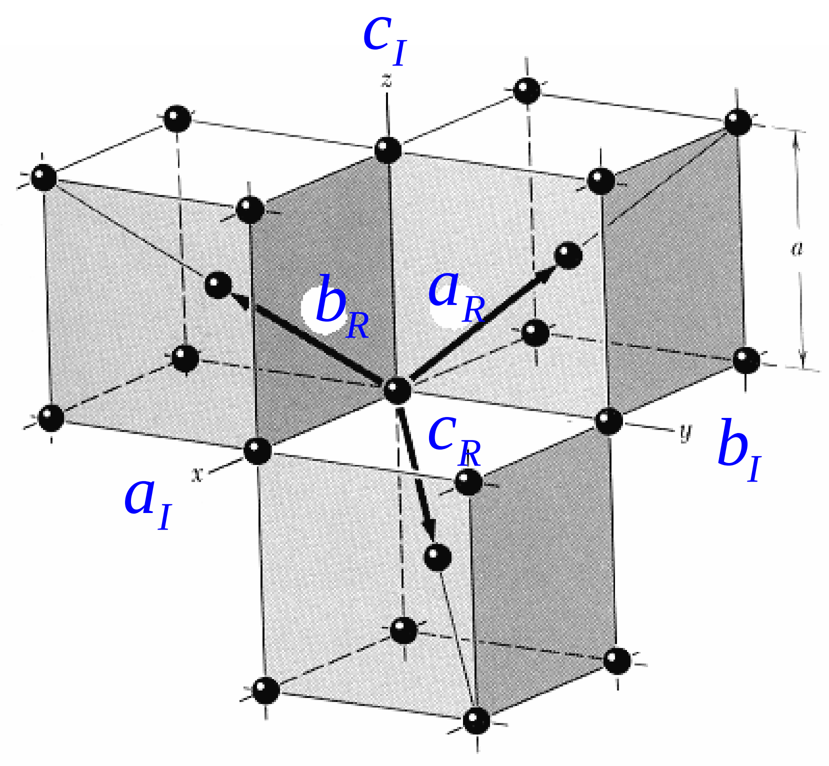


Fig. 6.4. (a) Plan of a cubic *I* crystal perpendicular to the *z*-axis and (b) pattern of reciprocal lattice points perpendicular to the *z*-axis. Note the cubic *F* arrangement of reciprocal lattice points in this plane.

Example

- BCC (body centered cubic)





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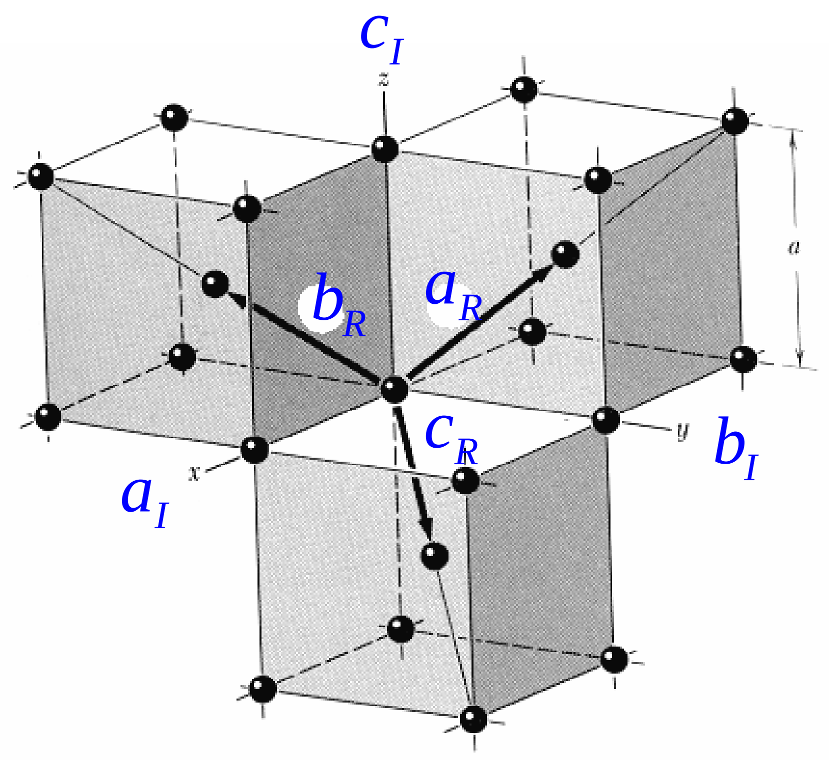
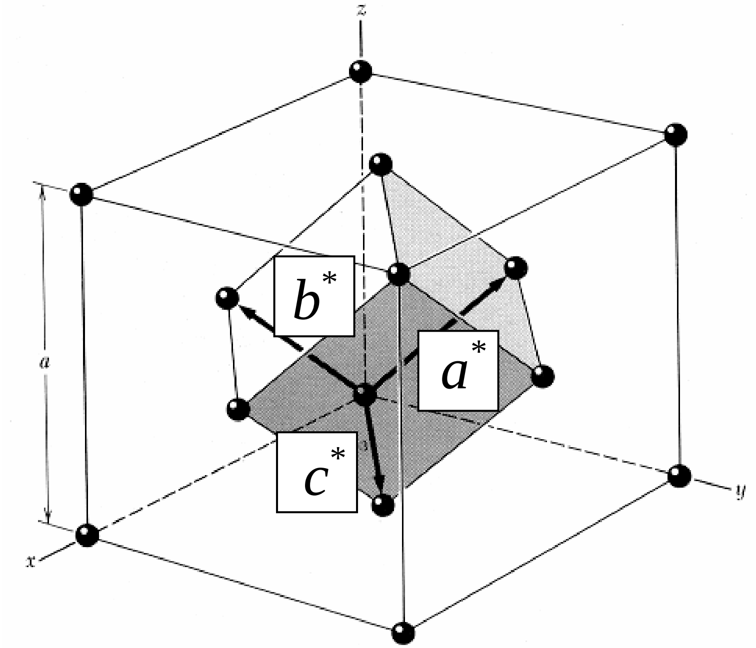
Example





$$a_R = \frac{1}{2}a(-\vec{x} + \vec{y} + \vec{z})$$

$$b_R = \frac{1}{2}a(\vec{x} - \vec{y} + \vec{z})$$

$$c_R = \frac{1}{2}a(\vec{x} + \vec{y} - \vec{z})$$

$$a^* = \frac{2\pi}{a}(\vec{y} + \vec{z})$$

$$b^* = \frac{2\pi}{a}(\vec{z} + \vec{x})$$

$$c^* = \frac{2\pi}{a}(\vec{x} + \vec{y})$$

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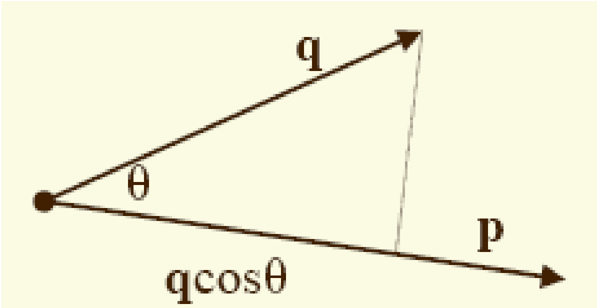
Metric Tensor

- consider two vectors $\vec{p}$ and $\vec{q}$:

$$\vec{p} = p_1\vec{a}_1 + p_2\vec{a}_2 + p_3\vec{a}_3, \qquad \vec{q} = q_1\vec{a}_1 + q_2\vec{a}_2 + q_3\vec{a}_3$$

$$\vec{p} = \sum_i p_i a_i, \qquad \vec{q} = \sum_j q_j a_j$$



- the dot product is defined as follows:

$$\vec{p}\bullet\vec{q} = \left|\vec{p}\right|\left|\vec{q}\right|\cos\theta = (\sum_i p_i a_i)\bullet(\sum_i q_i a_i) = \sum_i p_i q_j (a_i)\bullet(a_j)$$

$$= (p_1, p_2, p_3)\begin{pmatrix} \vec{a}\bullet\vec{a} & \vec{a}\bullet\vec{b} & \vec{a}\bullet\vec{c} \\ \vec{b}\bullet\vec{a} & \vec{b}\bullet\vec{b} & \vec{b}\bullet\vec{c} \\ \vec{c}\bullet\vec{a} & \vec{c}\bullet\vec{b} & \vec{c}\bullet\vec{c} \end{pmatrix}\begin{pmatrix} q_1 \\ q_2 \\ q_3 \end{pmatrix} = (p_1, p_2, p_3)G_{ij}\begin{pmatrix} q_1 \\ q_2 \\ q_3 \end{pmatrix}$$

Metric Tensor

- metric tensor $G_{ij} = \begin{pmatrix} \vec{a}\bullet\vec{a} & \vec{a}\bullet\vec{b} & \vec{a}\bullet\vec{c} \\ \vec{b}\bullet\vec{a} & \vec{b}\bullet\vec{b} & \vec{b}\bullet\vec{c} \\ \vec{c}\bullet\vec{a} & \vec{c}\bullet\vec{b} & \vec{c}\bullet\vec{c} \end{pmatrix}$

- a 3×3 matrix tensor contains all the geometric information about the unit cell

- example

$$\{2,3,4,90,60,90\} \Rightarrow G_{ij} = \begin{pmatrix} 4 & 0 & 4 \\ 0 & 9 & 0 \\ 4 & 0 & 16 \end{pmatrix}$$

표 1.4 각 결정축계에 대한 미터 행렬

결정축계	실격자	역격자
입 방	$\begin{pmatrix} a^2 & 0 & 0 \\ 0 & a^2 & 0 \\ 0 & 0 & a^2 \end{pmatrix}$	$\begin{pmatrix} \frac{1}{a^2} & 0 & 0 \\ 0 & \frac{1}{a^2} & 0 \\ 0 & 0 & \frac{1}{a^2} \end{pmatrix}$
정 방	$\begin{pmatrix} a^2 & 0 & 0 \\ 0 & a^2 & 0 \\ 0 & 0 & c^2 \end{pmatrix}$	$\begin{pmatrix} \frac{1}{a^2} & 0 & 0 \\ 0 & \frac{1}{a^2} & 0 \\ 0 & 0 & \frac{1}{c^2} \end{pmatrix}$
육 방	$\begin{pmatrix} a^2 & -\frac{1}{2}a^2 & 0 \\ -\frac{1}{2}a^2 & a^2 & 0 \\ 0 & 0 & c^2 \end{pmatrix}$	$\begin{pmatrix} \frac{4}{3a^2} & \frac{2}{3a^2} & 0 \\ \frac{2}{3a^2} & \frac{4}{3a^2} & 0 \\ 0 & 0 & \frac{1}{c^2} \end{pmatrix}$
능 면	$\begin{pmatrix} g_{11} & g_{12} & g_{12} \\ g_{12} & g_{11} & g_{12} \\ g_{12} & g_{12} & g_{11} \end{pmatrix}$ $g_{11}=a^2$ $g_{12}=a^2\cos\alpha$	$\begin{pmatrix} g^{11} & g^{12} & g^{12} \\ g^{12} & g^{11} & g^{12} \\ g^{12} & g^{12} & g^{11} \end{pmatrix}$ $g^{11}=\dfrac{1+\cos\alpha}{a^2(1-\cos\alpha)(1+2\cos\alpha)}$ $g^{12}=\dfrac{-\cos\alpha}{a^2(1-\cos\alpha)(1+2\cos\alpha)}$
사 방	$\begin{pmatrix} a^2 & 0 & 0 \\ 0 & b^2 & 0 \\ 0 & 0 & c^2 \end{pmatrix}$	$\begin{pmatrix} \frac{1}{a^2} & 0 & 0 \\ 0 & \frac{1}{b^2} & 0 \\ 0 & 0 & \frac{1}{c^2} \end{pmatrix}$
단 사 (주축이 b일 때)	$\begin{pmatrix} a^2 & 0 & ac\cos\beta \\ 0 & b^2 & 0 \\ ac\cos\beta & 0 & c^2 \end{pmatrix}$	$\begin{pmatrix} (a^*)^2 & 0 & a^*c^*\cos\beta^* \\ 0 & (b^*)^2 & 0 \\ a^*c^*\cos\beta^* & 0 & (c^*)^2 \end{pmatrix}$
삼 사	$\begin{pmatrix} a^2 & ab\cos\gamma & ac\cos\beta \\ ab\cos\gamma & b^2 & bc\cos\alpha \\ ac\cos\beta & bc\cos\alpha & c^2 \end{pmatrix}$	$\begin{pmatrix} (a^*)^2 & a^*b^*\cos\gamma^* & a^*c^*\cos\beta^* \\ a^*b^*\cos\gamma^* & (b^*)^2 & b^*c^*\cos\alpha^* \\ a^*c^*\cos\beta^* & b^*c^*\cos\alpha^* & (c^*)^2 \end{pmatrix}$

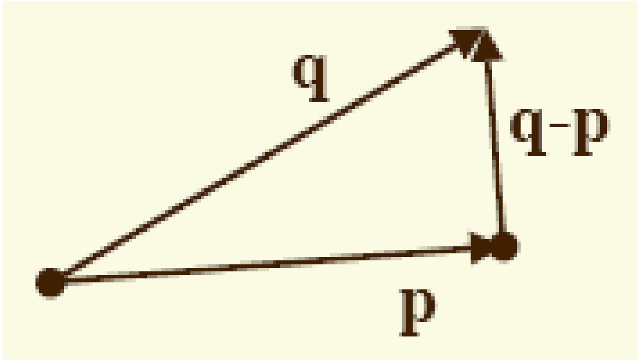
a^* 등에 대한 값은 앞절에 주었음.

Metric Tensor

- distance between two atoms:

$$D^2 = (\vec{q} - \vec{p}) \bullet (\vec{q} - \vec{p})$$

$$= (q_1 - p_1, q_2 - p_2, q_3 - p_3) G_{ij} \begin{pmatrix} q_1 - p_1 \\ q_2 - p_2 \\ q_3 - p_3 \end{pmatrix}$$



- bond angle $\cos\theta = \dfrac{\vec{p} \bullet \vec{q}}{\sqrt{\vec{p} \bullet \vec{p}}\sqrt{\vec{q} \bullet \vec{q}}}$

Example

- distance between 2,0,1 and 1,0,2
  in a monoclinic lattice {2,3,4,90,60,90}?

- angle between directions [210] and [102]
  in a monoclinic lattice {2,3,4,90,60,90}?

Crystallographic Education Online

Educational Resources

Aperiodic Crystallography

- QuasiTiler 3.0 by Geometry Center, University of Minnesota. QuasiTiler draws Penrose tilings and their generalizations.

Applied Crystallography

- The Study of Metals and Alloys by X-ray Powder Diffraction Methods. by H. Lipson