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}



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

Space lattice (공간격자)



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)













http://www.kings.edu/~chemlab/vrml/

- 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 1/21/32/3 \vec{uvw}

- lattice line, [uvw]
 - line- two points I: 000 231 → [231] II: 000 112 → [112] II': 100 212 → [112]

family <uvw>





* 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, $\overline{210} \rightarrow [210]$ opposite direction $\overline{130}$ and $\overline{130}$ A Family of Directions and Planes

 $- \langle 111 \rangle$ angular bracket $- \{100\}$ braces



*[111] square bracket

*(100) parentheses

- Lattice plane (Miller indices)



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



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

* 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

Equation of a rational intercept plane

M

X

$$\frac{x}{m} + \frac{y}{n} + \frac{z}{p} = 1$$

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

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

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

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

n y

* 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 [u₁v₁w₁] and [u₂v₂w₂] lie in the lattice plane (hkl) whose indices can be determined from the zonal equation:



 * The lattice planes (h₁k₁l₁) and (h₂k₂l₂) intersect in the lattice line [uvw]whose indices can be determined

$$h_1 u + k_1 v + l_1 w = 0$$
 $h_2 u + k_2 v + l_2 w = 0$



Direction vs. Planes of Same Indices



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}



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

$$\vec{a}^* = \frac{\vec{b} \times \vec{c}}{abc} \quad \vec{b}^* = \frac{\vec{c} \times \vec{a}}{abc} \quad \vec{c}^* = \frac{\vec{a} \times \vec{b}}{abc} \qquad \vec{a} \cdot \vec{a}^* = 1 \qquad \vec{a} \cdot \vec{b}^* = 0 \qquad \vec{a} \cdot \vec{c}^* = 0$$
$$\vec{b} \cdot \vec{a}^* = 0 \qquad \vec{b} \cdot \vec{b}^* = 1 \qquad \vec{b} \cdot \vec{c}^* = 0$$
$$\vec{c} \cdot \vec{a}^* = 0 \qquad \vec{c} \cdot \vec{b}^* = 0 \qquad \vec{c} \cdot \vec{c}^* = 1$$

Reciprocal lattice and interplanar spacing d_{hkl}



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

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

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



http://www.matter.org.uk/diffraction/geometry/2D_reciprocal_lattices.htm http://www.humboldt.edu/~gdg1/recip.html

For every real lattice there is an equivalent <u>reciprocal lattice</u>. A two dimension (2-D) real lattice is defined by two <u>unit cell vectors</u>, **a** and **b** inclined at an angle γ as shown below. The equivalent reciprocal lattice in reciprocal space is defined by two reciprocal vectors, **a**^{*} and **b**^{*}.

The reciprocal vectors are defined as follows:

- **a*** is of magnitude $1/d_{10}$ where d_{10} is the spacing of the (10) planes, and is perpendicular to **b**,
- **b*** is of magnitude $1/d_{01}$ where d_{01} is the spacing of the (01) planes, and is perpendicular to **a**.

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

Note: each point in the reciprocal lattice represents a set of planes.



square



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



In the lattice shown above, the reciprocal vectors are parallel to their corresponding real vectors. This is only true for the unit cells of certain crystal systems, which are they?

표 1.2 실격자와 역격자의 단위 수치간의 관계

$a^* = \frac{bc \sin \alpha}{V}$	$\cos \alpha^* = \frac{\cos \beta \cos \gamma - \cos \alpha}{\sin \beta \sin \gamma}$
$b^* = \frac{ca\sin\beta}{V}$	$\cos \beta^* = \frac{\cos \gamma \cos \alpha - \cos \beta}{\sin \gamma \sin \alpha}$
$c^* = \frac{ab\sin\gamma}{V}$	$\cos \gamma^* = \frac{\cos \alpha \cos \beta - \cos \gamma}{\sin \alpha \sin \beta}$
$a = \frac{b^* c^* \sin a^*}{V^*}$	$\cos \alpha = \frac{\cos \beta^* \cos \gamma^* - \cos \alpha^*}{\sin \beta^* \sin \gamma^*}$
$b = \frac{c^* a^* \sin \beta^*}{V^*}$	$\cos\beta = \frac{\cos\gamma^*\cos\alpha^* - \cos\beta^*}{\sin\gamma^*\sin\alpha^*}$
$c = \frac{a^* b^* \sin \gamma^*}{V^*}$	$\cos \gamma = \frac{\cos \alpha^* \cos \beta^* - \cos \gamma^*}{\sin \alpha^* \sin \beta^*}$
	$V^* = a^* b^* c^* \sqrt{1 - \cos^2 a^* - \cos^2 \beta^* - \cos^2 \gamma^* + 2\cos a^* \cos \beta^* \cos \gamma^*}$
	$V = abc \sqrt{1 - \cos^2 \alpha - \cos^2 \beta - \cos^2 \gamma + 2 \cos \alpha \cos \beta \cos \gamma}$

표 1.3 면간거리

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

Reciprocal Lattice and Interplanar Spacing d_{hkl}

- monoclinic P $a \neq b \neq c$ $\alpha = \gamma = 90^{\circ} \neq \beta$



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 a = b = c $\alpha = \beta = \gamma = 90^{\circ}$



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)





C. Kittel, Introduction to Solid State Physics

Example





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

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

$$\vec{p} = p_1 \vec{a} + p_2 \vec{b} + p_3 \vec{c}, \qquad \vec{q} = q_1 \vec{a} + q_2 \vec{b} + q_3 \vec{c} \qquad \vec{p} = (\vec{a} \quad \vec{b} \quad \vec{c}) \begin{pmatrix} p_1 \\ p_2 \end{pmatrix}$$

 p_3

- the dot product is defined as follows:

$$\vec{p} \cdot \vec{q} = p^{t} \cdot q$$

$$= (p_{1}, p_{2}, p_{3})(\vec{a}, \vec{b}, \vec{c}) \begin{pmatrix} \vec{a} \\ \vec{b} \\ \vec{c} \end{pmatrix} \begin{pmatrix} q_{1} \\ q_{2} \\ q_{3} \end{pmatrix}$$

$$= (p_{1}, p_{2}, p_{3}) \begin{pmatrix} \vec{a} \cdot \vec{a} & \vec{a} \cdot \vec{b} & \vec{a} \cdot \vec{c} \\ \vec{b} \cdot \vec{a} & \vec{b} \cdot \vec{b} & \vec{b} \cdot \vec{c} \\ \vec{c} \cdot \vec{a} & \vec{c} \cdot \vec{b} & \vec{c} \cdot \vec{c} \end{pmatrix} \begin{pmatrix} q_{1} \\ q_{2} \\ q_{3} \end{pmatrix} = (p_{1}, p_{2}, p_{3}) G_{ij} \begin{pmatrix} q_{1} \\ q_{2} \\ q_{3} \end{pmatrix}$$

Metric Tensor

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

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

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

	기 같이가게게 개인 가의 이걸	
설정국계 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	$\begin{pmatrix} g_{11} & g_{12} & g_{12} \\ g_{12} & g_{11} & g_{12} \\ g_{12} & g_{12} & g_{11} \end{pmatrix}$ $g_{11} = a^2$ $g_{12} = a^2 \cos a$	$ \begin{pmatrix} g^{11} & g^{12} & g^{12} \\ g^{12} & g^{11} & g^{12} \\ g^{12} & g^{12} & g^{12} \\ g^{12} & g^{12} & g^{11} \end{pmatrix} $ $ g^{11} = \frac{1 + \cos a}{a^2(1 - \cos a)(1 + 2\cos a)} $ $ g^{12} = \frac{-\cos a}{a^2(1 - \cos a)(1 + 2\cos a)} $
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	$\begin{pmatrix} a^2 & ab\cos\gamma & ac\cos\beta\\ ab\cos\gamma & b^2 & bc\cos\alpha\\ ac\cos\beta & bc\cos\alpha & c^2 \end{pmatrix}$	$\begin{pmatrix} (a^{*})^{2} & a^{*}b^{*}\cos\gamma^{*} & a^{*}c^{*}\cos\beta^{*} \\ a^{*}b^{*}\cos\gamma^{*} & (b^{*})^{2} & b^{*}c^{*}\cos\alpha^{*} \\ a^{*}c^{*}\cos\beta^{*} & b^{*}c^{*}\cos\alpha^{*} & (c^{*})^{2} \end{pmatrix}$

표 1.4 각 결정축계에 대한 미터 행렬

a* 등에 대한 값은 앞절에 주었음.

Metric Tensor

q-p

р

- distance between two atoms:

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

$$= (q_{1} - p_{1}, q_{2} - p_{2}, q_{3} - p_{3})G_{ij}\begin{pmatrix}q_{1} - p_{1}\\q_{2} - p_{2}\\q_{3} - p_{3}\end{pmatrix}$$

- bond angle $\cos \theta = \frac{p \cdot q}{\sqrt{\vec{p} \cdot \vec{p}} \sqrt{\vec{q} \cdot \vec{q}}}$

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}?

http://journals.iucr.org/cww-top/edu.index.html



Crystallographic Education Online

Educational Resources

Aperiodic Crystallography

•<u>QuasiTiler 3.0</u> by Geometry Center, University of Minnesota. QuasiTiler draws Penrose tilings and their generalizations.

Applied Crystallography

•<u>The Study of Metals and Alloys by X-ray Powder Diffraction Methods.</u> by H. Lipson



Which lattice line is common to the lattice planes (101) and $(\overline{1}12)$?