3-2. Symmetry in Crystal

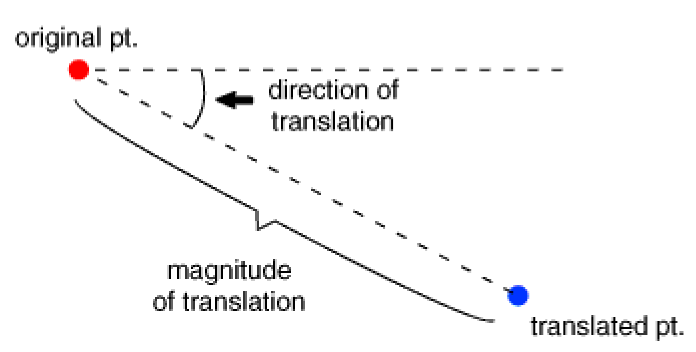
Contents

- Translation symmetry
- Rotation symmetry
- Mirror symmetry
- Inversion symmetry

- **Symmetry** is the preservation of form and configuration across an point, a line, or a plane.
- In informal terms, symmetry is the ability to take a shape and match it exactly to another shape.
- The techniques that are used to "take a shape and match it exactly to another" are called **transformations** and include **translations**, **rotations,** **mirror(reflections)**, and **inversion symmetry**.

Translations and Translational Symmetry

- The most simple type of symmetry is **translational symmetry** which results from the transformation called **translation**.
- Translation is just a fancy term for "move." When a shape is moved, two specifications are needed: a **direction** and **magnitude**. Direction can be measured in degrees (e.g., 30 degrees north of east), while magnitude can be measured in inches (e.g., 2 inches) or some other unit of length.



A simple translation of a point (red) to form another point (blue). Two specifications are needed: direction and magnitude

- For 1-dimension, lattice vector can be expressed by

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

where u is integer and $\vec{a}$ the fundamental lattice translation vector.

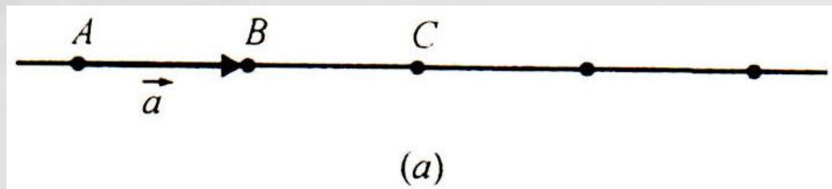
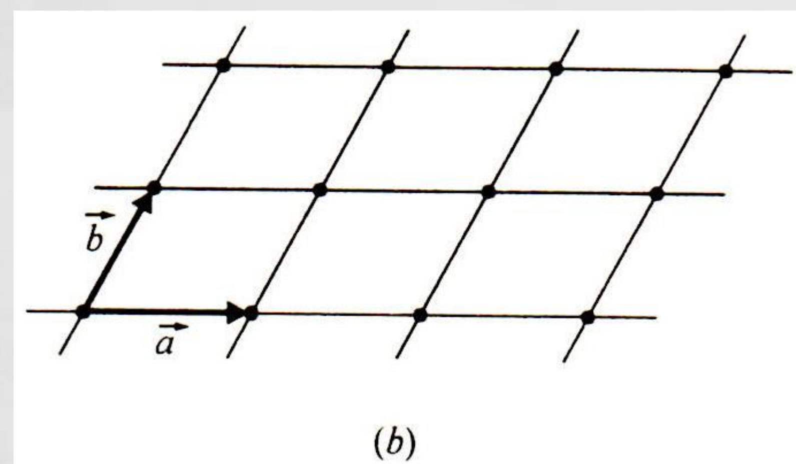


그림 3-6 병진 대칭. (a) 1 차원($\vec{r} = u\vec{a}$),

- For 2-dimension, lattice vector can be expressed by

$$\vec{r} = u\vec{a} + v\vec{b}$$

where u and v are integers and $\vec{a}, \vec{b}$ the fundamental lattice translation vectors.

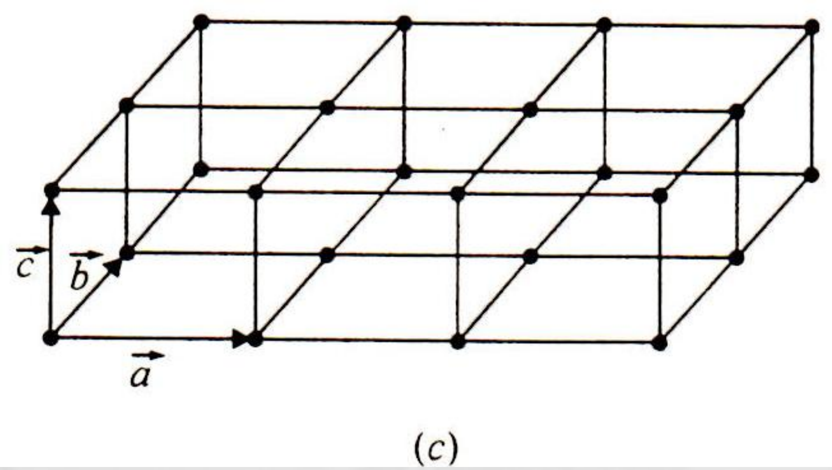


(b) 2 차원($\vec{r} = u\vec{a} + v\vec{b}$)

- For 3-dimension, lattice vector can be expressed by

$$\vec{r} = u\vec{a} + v\vec{b} + w\vec{c}$$

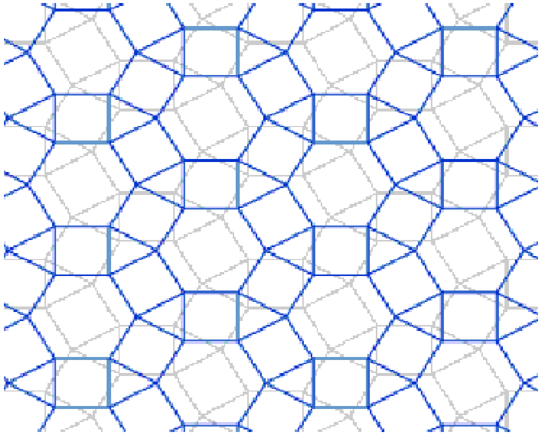
where *u, v and w* is integers and $\vec{a}, \vec{b}, \vec{c}$ the fundamental lattice translation vector.



(c) 3 차원($\vec{r} = u\vec{a} + v\vec{b} + w\vec{c}$)

The volume of unit cell, **parallelepiped,** is given by

$$\Omega = \vec{a} \cdot [\vec{b} \times \vec{c}]$$



This tessellation has translational symmetry; after moving a copy in a certain direction and with a certain magnitude, you find that the copy matches exactly the original

Real examples of translational symmetry:

Rotational Symmetry

- The rotational symmetry is a symmetry factor that after the system rotates for a point or an axis, the system is on the same situation.
- The available rotation angles are 360° , 180° , 120° , 90° , 60° .

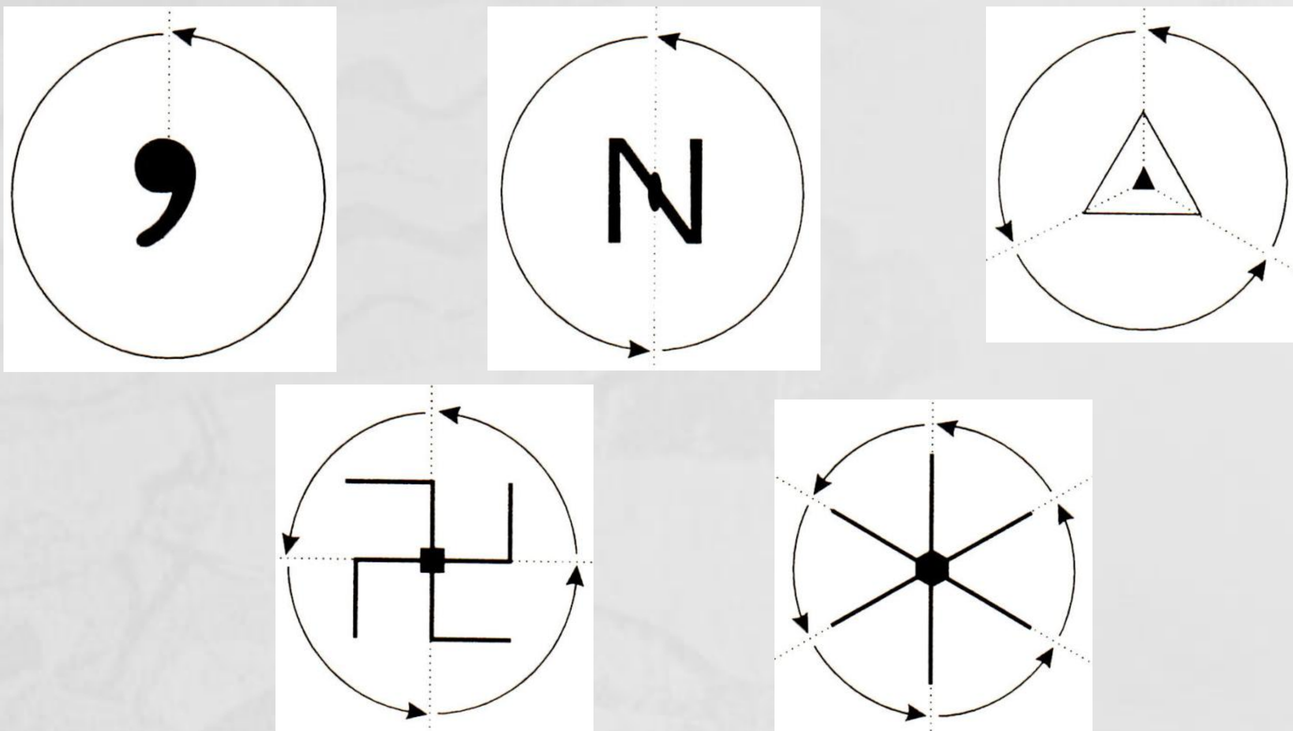


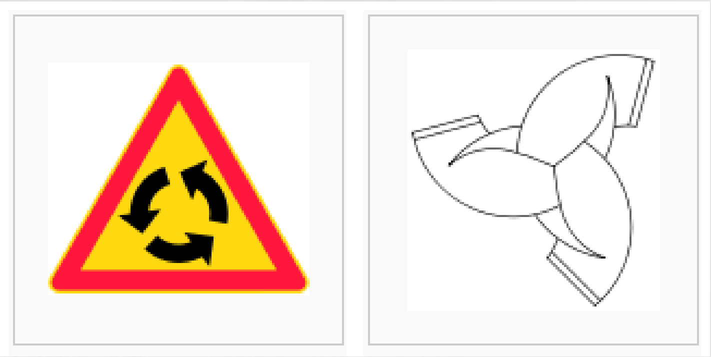
그림 3-7 1-중, 2-중, 3-중, 4-중, 6-중 회전 대칭축

n-fold rotational symmetry

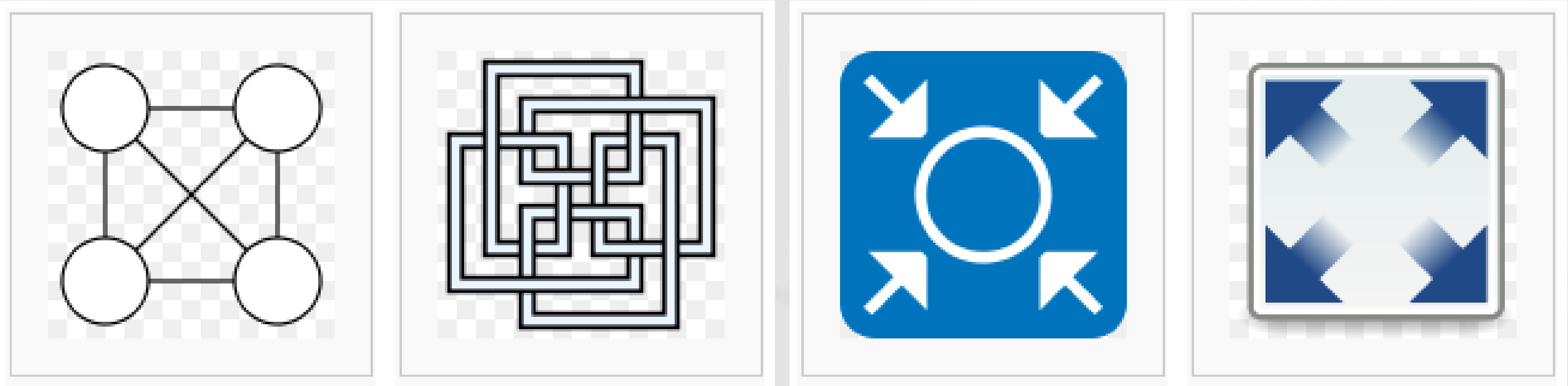
- **Rotational symmetry of order *n***, also called ***n*-fold rotational symmetry**, or **discrete rotational symmetry of the nth order**, with respect to a particular point (in 2D) or axis (in 3D) means that rotation by an angle of 360° /n (180° , 120° , 90° , 72° , 60° , 51 3/7 ° , etc.) does not change the object.
- The notation for *n*-fold symmetry is C_n or simply "*n*". The actual symmetry group is specified by the point or axis of symmetry, together with the *n*.
- The fundamental domain is a sector of 360° /n.
- Examples without additional reflection symmetry:
- *n* = 2, 180° : the dyad, quadrilaterals with this symmetry are the parallelograms; other examples: letters Z, N, S; apart from the colors: yin and yang
- *n* = 3, 120° : triad, triskelion, Borromean rings; sometimes the term *trilateral symmetry* is used;
- *n* = 4, 90° : tetrad, swastika
- *n* = 6, 60° : hexad, raelian symbol, new version

- Examples of 2-fold rotational symmetry

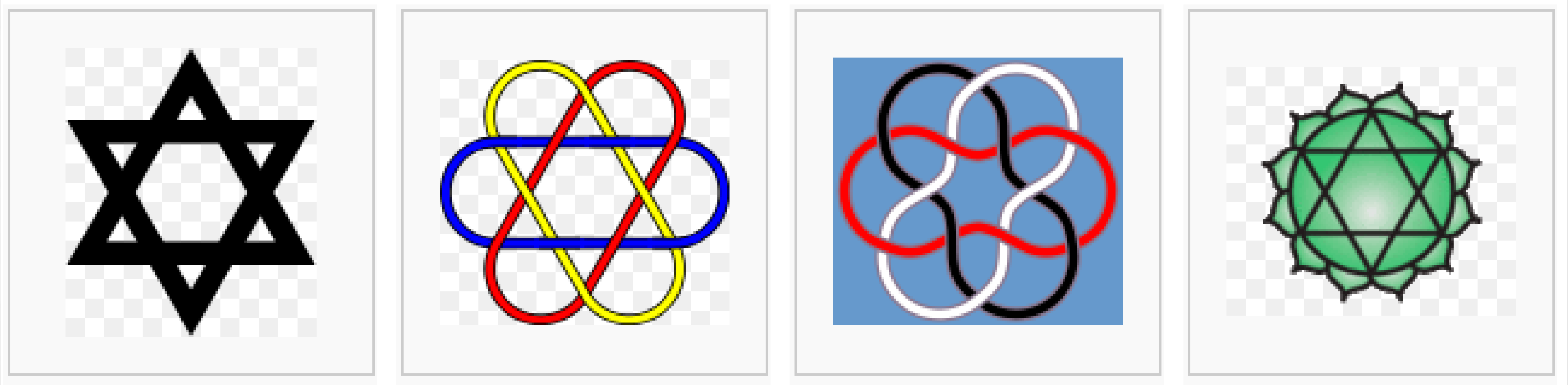
- Examples of 3-fold rotational symmetry



- Examples of 4-fold rotational symmetry

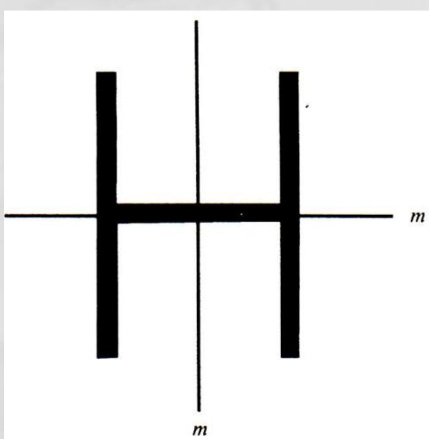


- Examples of 6-fold rotational symmetry



Mirror Symmetry(경영 대칭)

- **Reflectional symmetry**, **line symmetry**, **mirror symmetry**, **mirror-image symmetry**, or **bilateral symmetry** is symmetry with respect to reflection. That is, a figure which does not change upon undergoing a reflection has reflectional symmetry.
- **Bilateral symmetry** is the symmetry everybody is aware of, and to many people this is symmetry itself. Bilateral symmetry occurs when two halves of a whole are each other's mirror images. Accordingly, bilateral symmetry is also called *mirror symmetry*.



- Examples of mirror symmetry

그림 3-8 경영 대칭의 예

3-2-1 Symmetry factors in crystal

- All the crystals should simultaneously satisfy the translation, rotation and mirror symmetries.
- Therefore, there can be several fold symmetry including n=1, 2, 3, 4, 6.
- Let's discuss about this property using Fig. 3-10.

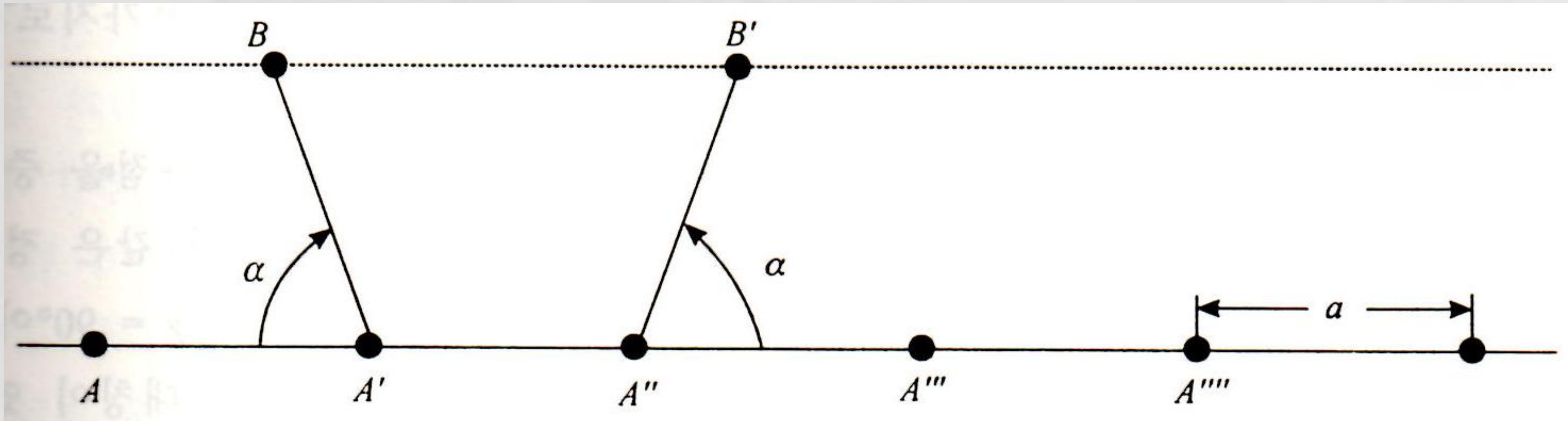


그림 3-10 2차원 격자에서의 회전대칭.

그러면 어떻게 5가지 대칭축이 얻어지는지 알아보기 위해, 그림 3-10에 있는 2차원의 격자를 생각하여 여기에 회전 대칭이 있을 때를 살펴보자. 여기서 격자점을 A, A', A'', A''', A'''', …라 하고 AA' 방향으로 제일 짧은 기본 격자 병진 벡터를 $\vec{a}$라 하자. 그리고, 이 격자에서 각 격자점에 평면에 수직하게 n-중 대칭이 있다고 하자. 그러면 격자점 A'에서 격자점 A을 회전각 $\alpha = \angle AA'B = 360°/n$로 회전한 점 B 또한 격자점이 되어야 한다. A'' 점도 격자점이므로 A''에도 n-중 회전 대칭축이 있어 그림에서 격자점 A'''을 회전각 α로 회전한 점 B' 또한 격자점이 되어야 한다. 그러면 점 B, B'은 AA'에 평행한 선 위에 있는 격자점이 된다. 격자점이면 식 (3-1)을 만족하여

$$BB' = ua \tag{3-5}$$

이어야 하고 여기서 u는 정수이다.

그림 3-10으로부터 BB'은 $(a - 2a\cos\alpha)$이므로

$$a - 2a\cos\alpha = ua \tag{3-6}$$

이고,

$$\cos\alpha = \frac{1-u}{2} \tag{3-7}$$

이다. u가 정수이고 $|\cos\alpha| \le 1$이므로

$$-1 \le \cos\alpha = \frac{1-u}{2} \le 1 \tag{3-8}$$

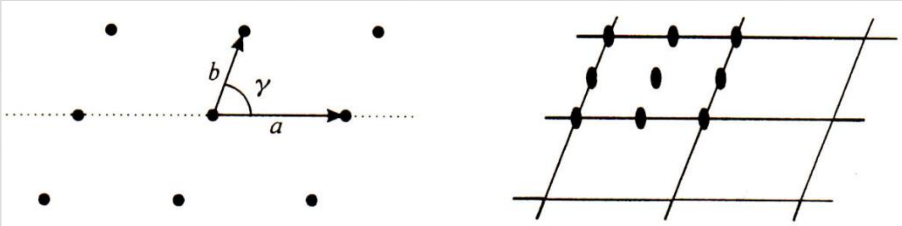
이고, 여기서 가능한 u의 값은 −1, 0, 1, 2, 3이 된다. 이 u에 대해 회전각을 구하면 표 3-1이 되어 결정에서 가능한 회전 대칭은 단중, 2-중, 3-중, 4-중, 6-중 대칭의 5가지 뿐임을 확인할 수 있다.

표 3-1 다섯가지 회전 대칭을 구하는 식의 해.

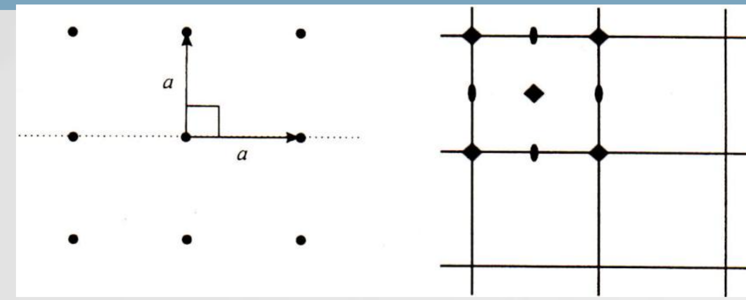
u	−1	0	1	2	3
$\cos\alpha$	1	1/2	0	−1/2	−1
α	0°	60°	90°	120°	180°

2 차원에서 대칭 요소를 추가하지 않고도 만들어지는 기본 격자는 평행사변형으로 된 격자로 평행사변형(parallelogram 또는 oblique) 격자라 한다. 평행사변형에서 이웃하는 두 변의 길이는 a, b 로 다르고 사이각 γ는 임의의 각이다. 평행사변형 격자는 표 3-1 에서 u 가 −1 또는 3, 즉 α = 0° 또는 180°인 경우에 해당되며 이들 회전각을 만족한다.

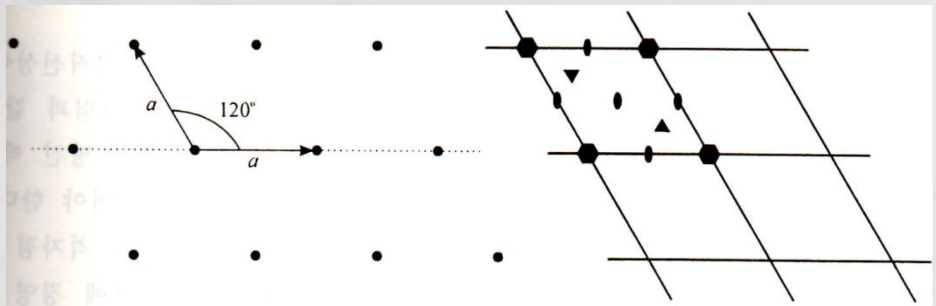
그림 3-11(a)는 평행사변형 격자를 그린 것으로 2 차원 격자면에 수직한 2-중 대칭축이 있음을 보여 준다. 이보다 대칭이 더 높은 대칭축은 존재하지 않는다. 이 격자에는 오른쪽에 표시한 것과 같이 모든 격자점, 각 변의 중점과 단위포의 중심에서 2-중 대칭을 나타낸다. 3 차원에서 모든 격자점이 대칭 중심인 것과 마찬가지로 2 차원 격자에서 격자점은 모두 격자면에 수직한 2-중 대칭을 지닌다.



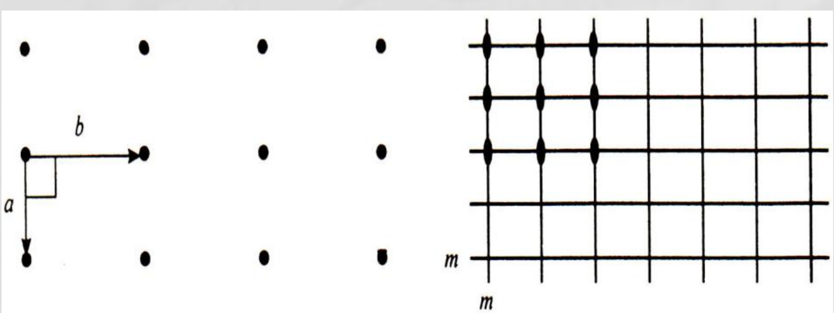
(a)



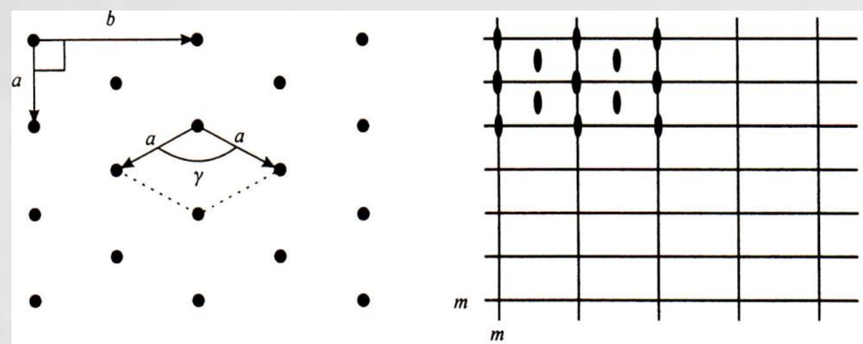
(b)



(c)



(d)

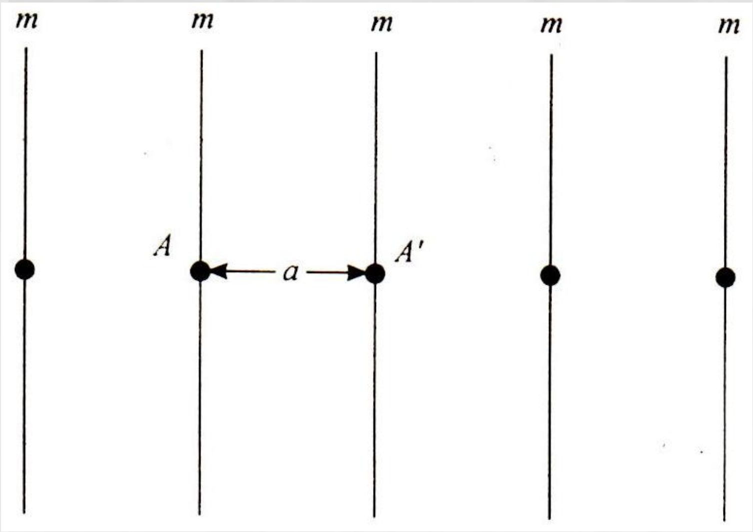


(e)

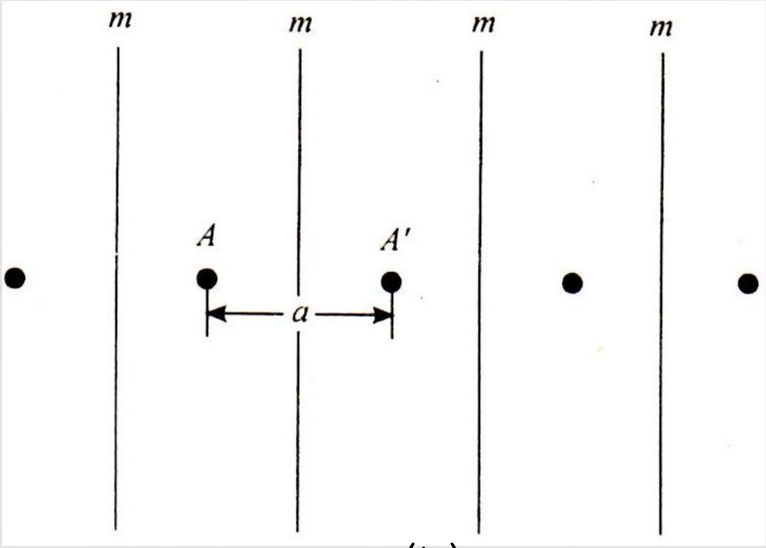
그림 3-11 5가지 2차원 격자와 대칭

Reflection symmetry in crystal

그림 3-13 에서 보여준 바와 같이 2 차원에서 경영 대칭면과 병진 대칭을 동시에 만족하는 배열은 2 가지가 있다. 그림 3-13 의 위 그림에 해당하는 격자가 바로 그림 3-11(*d*)에 있는 직사각형(rectangular) 격자이다. 직사각형 단위포에서 *a* 와 *b* 는 반드시 같을 필요는 없고 $\gamma = 90°$이다. 오른쪽 그림과 같이 경영 대칭면의 교차점에는 2-중 대칭이 있다.



(a)



(b)

그림 3-12 격자에서의 경영대칭. (a) 격자점 위의 경영 대칭면.
(b) 격자점과 격자점의 가운데에 있는 경영 대칭면.

3-3 Crystal Systems

- In crystallography, the terms **crystal system**, **crystal family**, and **lattice system** each refer to one of several classes of space groups, lattices, point groups, or crystals. Informally, two crystals tend to be in the same crystal system if they have similar symmetries, though there are many exceptions to this.
- Crystal systems, crystal families, and lattice systems are similar but slightly different, and there is widespread confusion between them: in particular the trigonal crystal system is often confused with the rhombohedral lattice system, and the term "crystal system" is sometimes used to mean "lattice system" or "crystal family".

- Space groups and crystals are divided into 7 crystal systems according to their point groups, and into 7 lattice systems according to their Bravais lattices.
- Five of the crystal systems are essentially the same as five of the lattice systems, but the hexagonal and trigonal crystal systems differ from the hexagonal and rhombohedral lattice systems.
- The six crystal families are formed by combining the hexagonal and trigonal crystal systems into one hexagonal family, in order to eliminate this confusion.

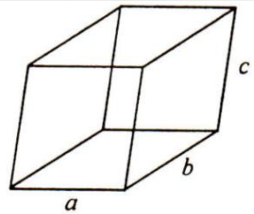
- The relation between three-dimensional crystal families, crystal systems, and lattice systems is shown in the following table:

<table>
<tr><th>Crystal family</th><th>Crystal system</th><th>Required symmetries of point group</th><th>point groups</th><th>space groups</th><th>bravais lattices</th><th>Lattice system</th></tr>
<tr><td colspan="2">Triclinic</td><td>None</td><td>2</td><td>2</td><td>1</td><td>Triclinic</td></tr>
<tr><td colspan="2">Monoclinic</td><td>1 twofold axis of rotation or 1 mirror plane</td><td>3</td><td>13</td><td>2</td><td>Monoclinic</td></tr>
<tr><td colspan="2">Orthorhombic</td><td>3 twofold axes of rotation or 1 twofold axis of rotation and two mirror planes.</td><td>3</td><td>59</td><td>4</td><td>Orthorhombic</td></tr>
<tr><td colspan="2">Tetragonal</td><td>1 fourfold axis of rotation</td><td>7</td><td>68</td><td>2</td><td>Tetragonal</td></tr>
<tr><td rowspan="3">Hexagonal</td><td rowspan="2">Trigonal</td><td rowspan="2">1 threefold axis of rotation</td><td rowspan="2">5</td><td>7</td><td>1</td><td>Rhombohedral</td></tr>
<tr><td>18</td><td rowspan="2">1</td><td rowspan="2">Hexagonal</td></tr>
<tr><td>Hexagonal</td><td>1 sixfold axis of rotation</td><td>7</td><td>27</td></tr>
<tr><td colspan="2">Cubic</td><td>4 threefold axes of rotation</td><td>5</td><td>36</td><td>3</td><td>Cubic</td></tr>
<tr><td>Total: 6</td><td>7</td><td></td><td>32</td><td>230</td><td>14</td><td>7</td></tr>
</table>

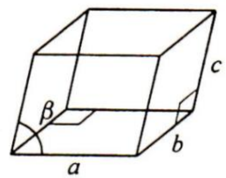
- The crystal systems can be classified with the three axes a, b, c, and the angles α, β, γ, between axes in 3-dimensional **parallelepiped.**

그림 3-17 7 결정계

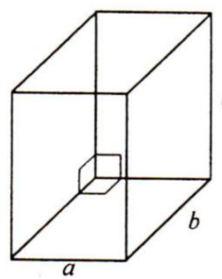
삼사정 $a \neq b \neq c,\ \alpha \neq \beta \neq \gamma$



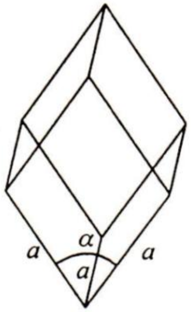
단사정 $a \neq b \neq c,\ \alpha = \gamma = 90^{\circ} \neq \beta$



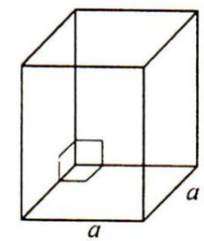
사방정 $a \neq b \neq c,\ \alpha = \beta = \gamma = 90^{\circ}$



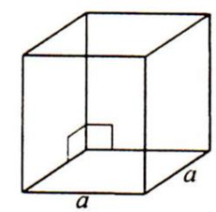
삼방정 $a = b = c,\ \alpha = \beta = \gamma \neq 90^{\circ} < 120^{\circ}$



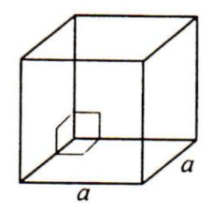
정방정 $a = b \neq c,\ \alpha = \beta = \gamma = 90^{\circ}$



육방정 $a = b \neq c,\ \alpha = \beta = 90^{\circ},\ \gamma = 120^{\circ}$



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



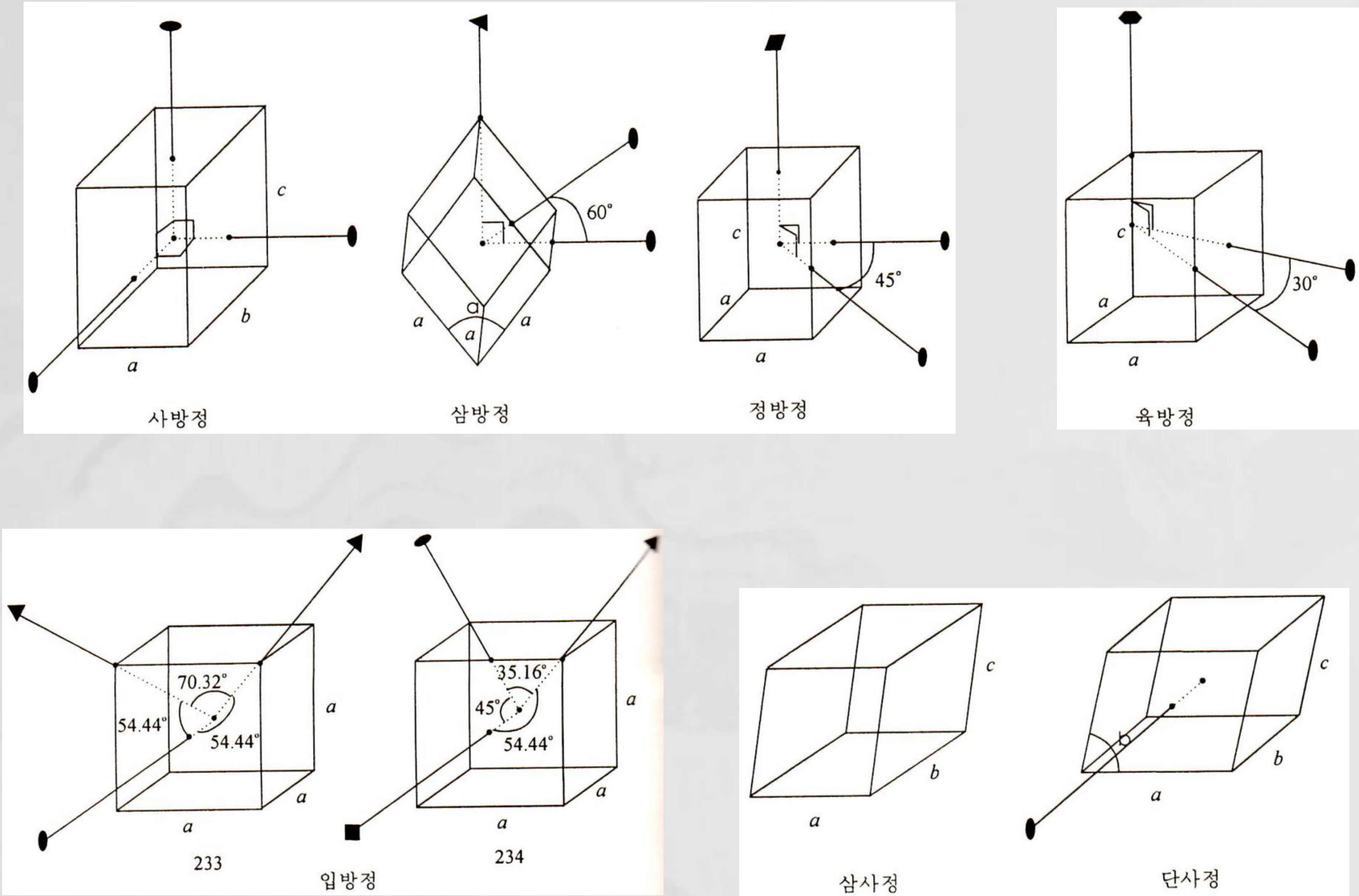


Fig. 3-18 shows the symmetry axes existed in crystal systems.

Table 3-3 describes the axes lengths, angles between axes and necessary symmetry factor for each crystal system.

표 3-3 7 결정계로 나눠지는 각 평행육면체의 축 길이, 축간 각, 필수 대칭 요소.

계	축 길이	축간 각	필수 대칭 요소
삼사정	$a \neq b \neq c$	$\alpha \neq \beta \neq \gamma$	없음
단사정	$a \neq b \neq c$	$\alpha = \gamma = 90° \neq \beta$	2-중 회전축 1 개
사방정	$a \neq b \neq c$	$\alpha = \beta = \gamma = 90°$	2-중 회전축 3 개(서로 수직)
삼방정	$a = b = c$	$\alpha = \beta = \gamma < 120°$	3-중 회전축 1 개
정방정	$a = b \neq c$	$\alpha = \beta = \gamma = 90°$	4-중 회전축 1 개
육방정	$a = b \neq c$	$\alpha = \beta = 90°,\ \gamma = 120°$	6-중 회전축 1 개
입방정	$a = b = c$	$\alpha = \beta = \gamma = 90°$	3-중 회전축 4 개(대각선 방향)