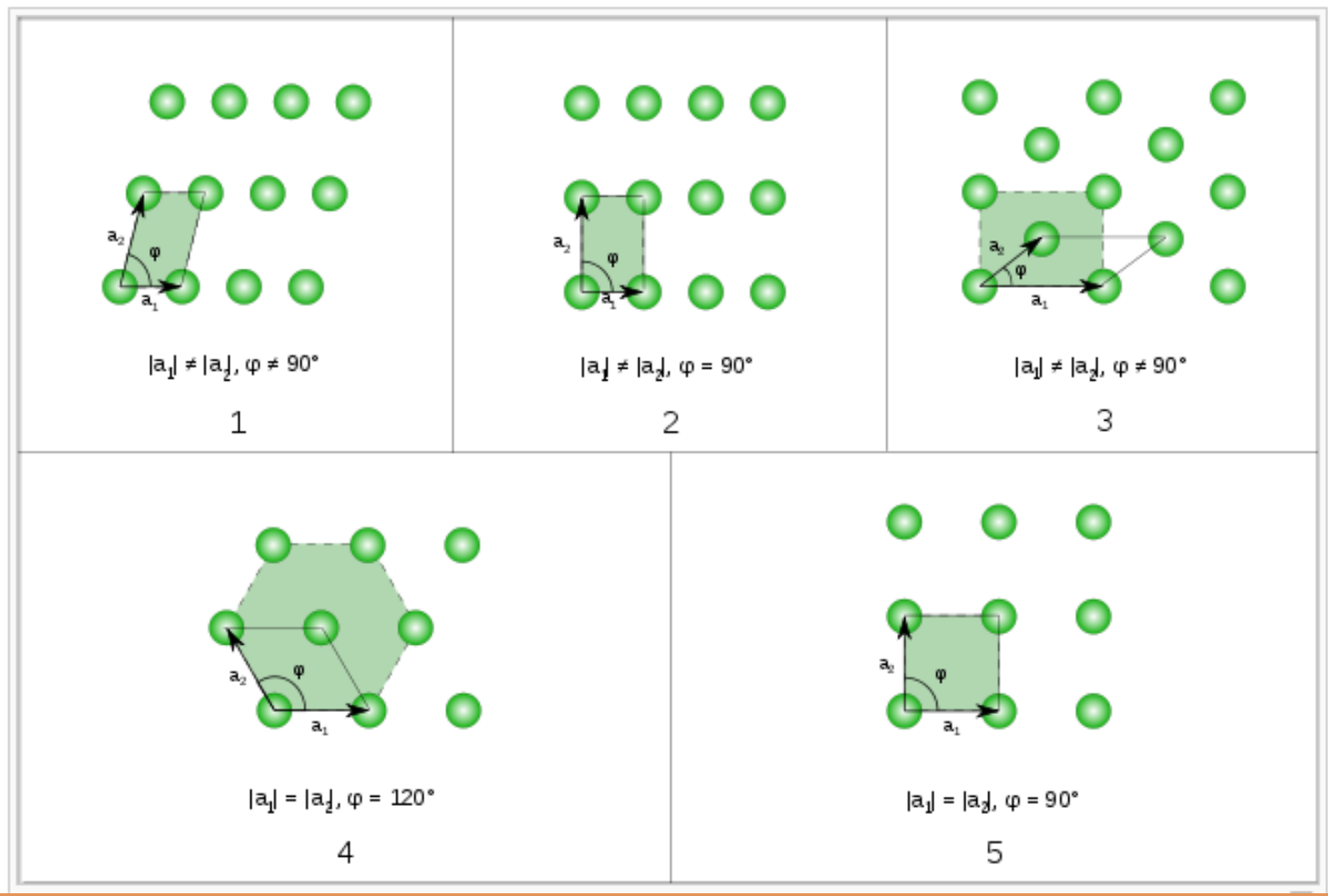
3-4 Bravais Lattice

- In geometry and crystallography, a **Bravais lattice**, studied by Auguste Bravais (1850),[1] is an infinite array of discrete points generated by a set of discrete translation operations described by:
- where n_i are any integers and $\mathbf{a_i}$ are known as the basis vectors which lie in different planes and span the lattice. This discrete set of vectors must be closed under vector addition and subtraction. For any choice of position vector **R**, the lattice looks exactly the same.
- A crystal is made up of a periodic arrangement of one or more atoms (the *basis*) repeated at each lattice point. Consequently, the crystal looks the same when viewed from any of the lattice points.
- Two Bravais lattices are often considered equivalent if they have isomorphic symmetry groups. In this sense, there are 14 possible Bravais lattices in three-dimensional space.

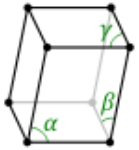
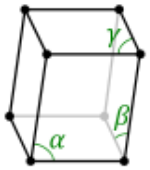
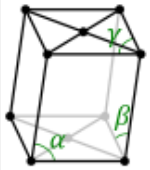
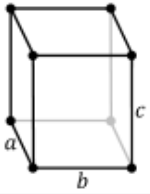
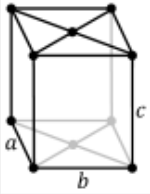
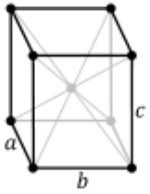
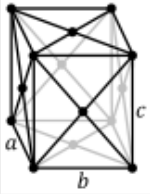
Bravais lattices in at most 2 dimensions

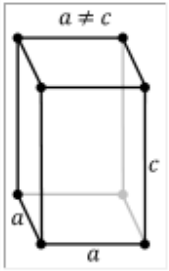
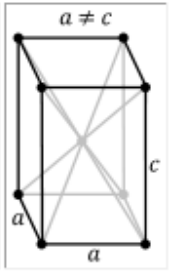
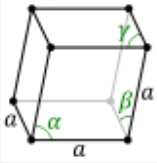
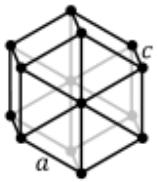
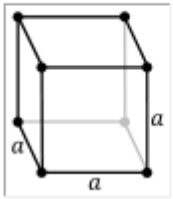
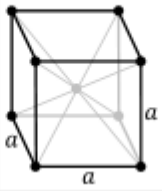
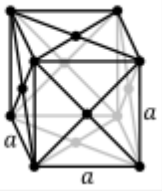
- In two dimensions, there are five Bravais lattices. They are oblique, rectangular, centered rectangular, hexagonal, and square.



Bravais lattices in 3 dimensions

- The 14 Bravais lattices in 3 dimensions are arrived at by combining one of the seven lattice systems (or axial systems) with one of the lattice centerings. Each Bravais lattice refers to a distinct lattice type.
- The lattice centerings are:
- Primitive centering (P): lattice points on the cell corners only
- Body centered (I): one additional lattice point at the center of the cell
- Face centered (F): one additional lattice point at center of each of the faces of the cell
- Base centered (A, B or C): one additional lattice point at the center of each of one pair of the cell faces.

The 7 lattice systems	The 14 Bravais lattices			
triclinic	P $\alpha, \beta, \gamma \neq 90°$ 			
monoclinic	P $\alpha \neq 90°$ $\beta, \gamma = 90°$ 	C $\alpha \neq 90°$ $\beta, \gamma = 90°$ 		
orthorhombic	P $a \neq b \neq c$ 	C $a \neq b \neq c$ 	I $a \neq b \neq c$ 	F $a \neq b \neq c$ 

tetragonal	P $a \neq c$ 	I $a \neq c$ 
rhombohedral	P $\alpha=\beta=\gamma \neq 90°$ 	
hexagonal	P 	
cubic	P (pcc) 	I (bcc) 	F (fcc) 

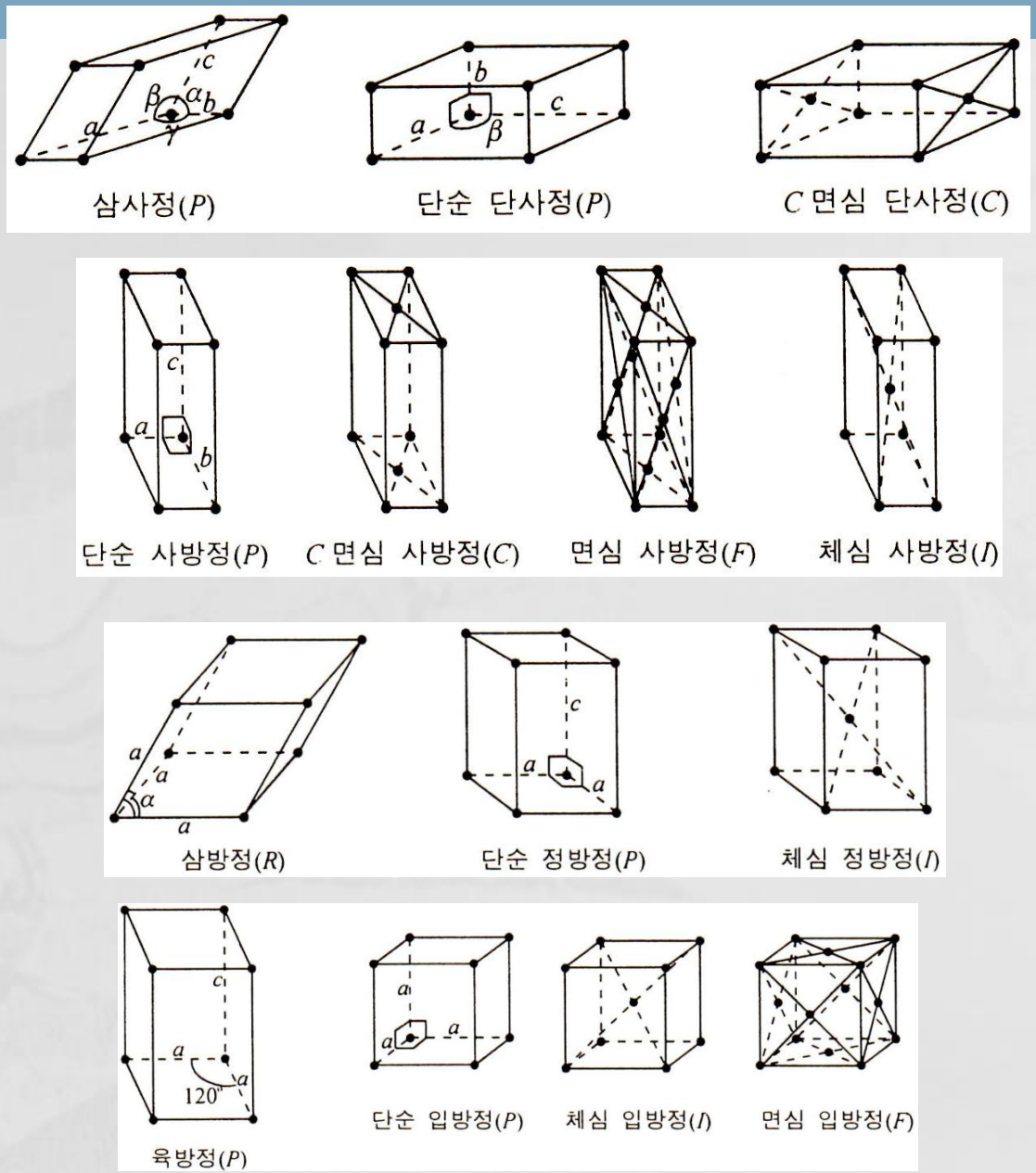


그림 3-20 결정에서 분류 가능한 14개의 브라배 공간 격자.

- The volume of the unit cell can be calculated by evaluating $\mathbf{a} \cdot \mathbf{b} \times \mathbf{c}$ where **a**, **b**, and **c** are the lattice vectors. The volumes of the Bravais lattices are given below:

Lattice system	Volume
Triclinic	$abc\sqrt{1 - \cos^2\alpha - \cos^2\beta - \cos^2\gamma + 2\cos\alpha\cos\beta\cos\gamma}$
Monoclinic	$abc \ \sin\alpha$
Orthorhombic	abc
Tetragonal	a^2c
rhombohedral	$a^3\sqrt{1 - 3\cos^2\alpha + 2\cos^3\alpha}$
Hexagonal	$\frac{\sqrt{3}\ a^2c}{2}$
Cubic	a^3

3-5 Lattice plane and direction

Lattice plane and direction in 2-dim.

- Figure 3-24 shows the 2-dim. Rectangular net with lattice constant *a* and *b*.

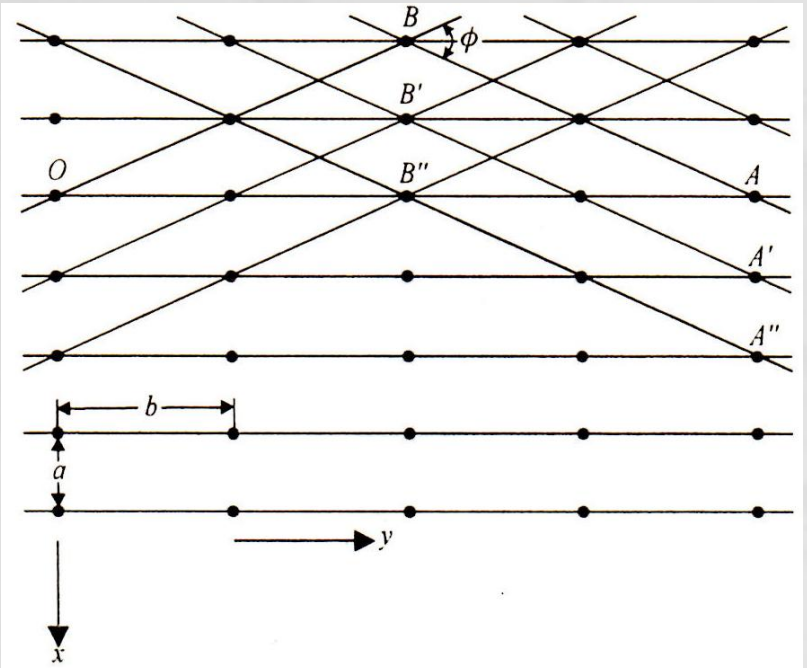


그림 3-24 격자 상수가 *a*, *b* 인 2 차원 직사각형 망목.

- In the figure 3-24, the distance between the lines is determined by the angle between lines.
- And the distance between lines can be calculated by

$$d = \frac{ab}{2\sqrt{a^2 + b^2}} \qquad \textbf{(3-18)}$$

- The angle between the segments OB and AB can be expressed by

$$2\tan^{-1}(b/a)$$

that depends on *a* and *b*.

Lattice plane and direction in 3-dim.

- In 3 dimensional crystal, lattice points are arrayed in 3-dimensional space, if we connect any of 2 lattice points, we can get lattice direction. And if we connect any of 3 lattice points(those are not on the same line), we can get lattice plane.
- Generally, we are using 'Miller index' to express the direction and plane of crystal.

Miller indices are a notation system in crystallography for planes and directions in crystal (Bravais) lattices.
In particular, a family of lattice planes is determined by three integers *ℓ*, *m*, and *n*, the *Miller indices*. They are written (hkl), and each index denotes a plane orthogonal to a direction (h, k, l) in the basis of the reciprocal lattice vectors. By convention, negative integers are written with a bar, as in 3 for −3. The integers are usually written in lowest terms, i.e. their greatest common divisor should be 1. Miller index 100 represents a plane orthogonal to direction *ℓ*; index 010 represents a plane orthogonal to direction *m*, and index 001 represents a plane orthogonal to *n*.

How can we calculate the Miller Index

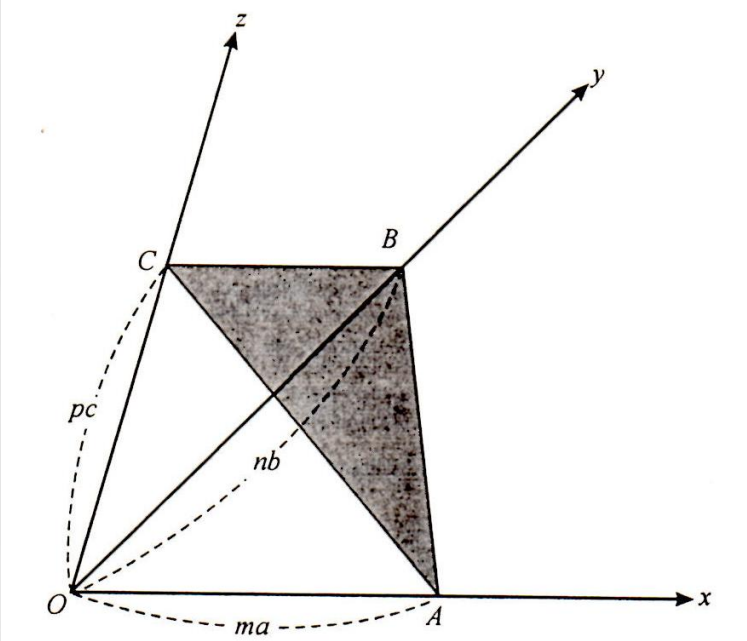


그림 3-25 격자면 *ABC*를 밀러 지수로 나타내는 방법.

- As shown in Fig. 3-25, the lattice plane intersect the x, y, z, axes at ma, nb, and pc, respectively.
- Step 1: Identify the intercepts on the x- , y- and z- axes.
- Step 2 : Specify the intercepts in fractional co-ordinates
- Step 3 : Take the reciprocals of the fractional intercepts.
  Take the reciprocal (inverse) of the coefficients of each intercepts m, n, and p. That is 1/m, 1/n, and 1/p.
- By multiplying the common multiple of m, n, and p to 1/m, 1/n and 1/p to make prime numbers h, k, and l, respectively.
- Then, (hkl) is the expression for the lattice plane of ABC shown in Fig. 3-25.

- For example, for the case of A=1a, B=2b and C=(1/3)c as shown in Fig. 3-26, we can calculate the Miller index as following.
- Take the coefficients, 1, 2, 1/3
- Multiply 2(the common multiple of 1, 2, and 1/3 multiple) to 1, 1/2 and 3, then we can get the number set 2, 1, and 6.
- Therefore, (2 1 6) is the Miller index of the given plane.

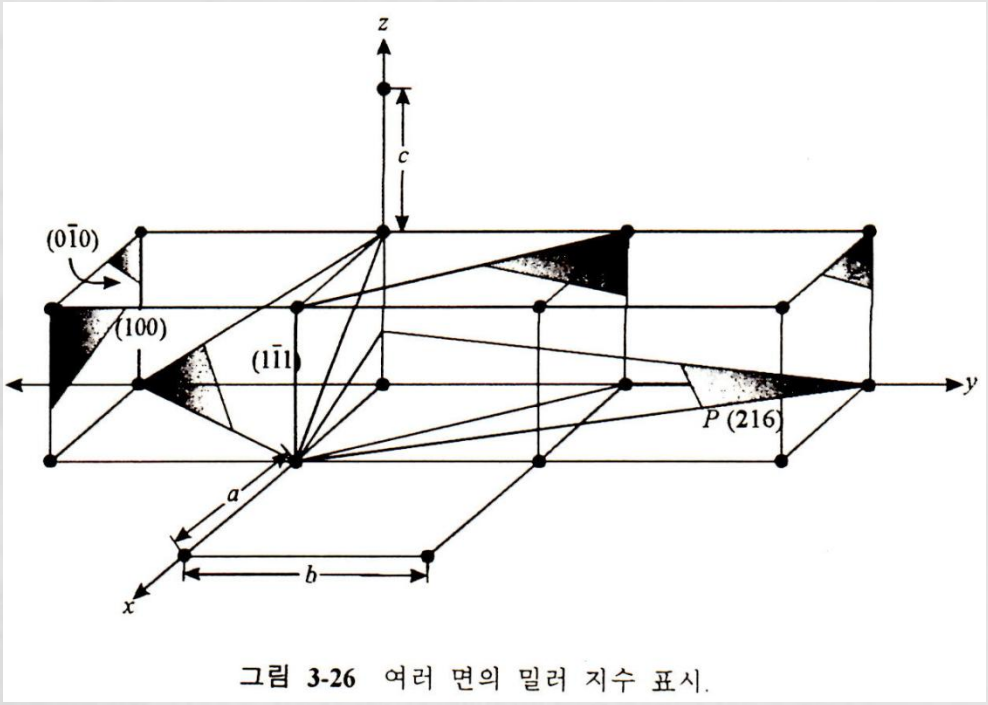
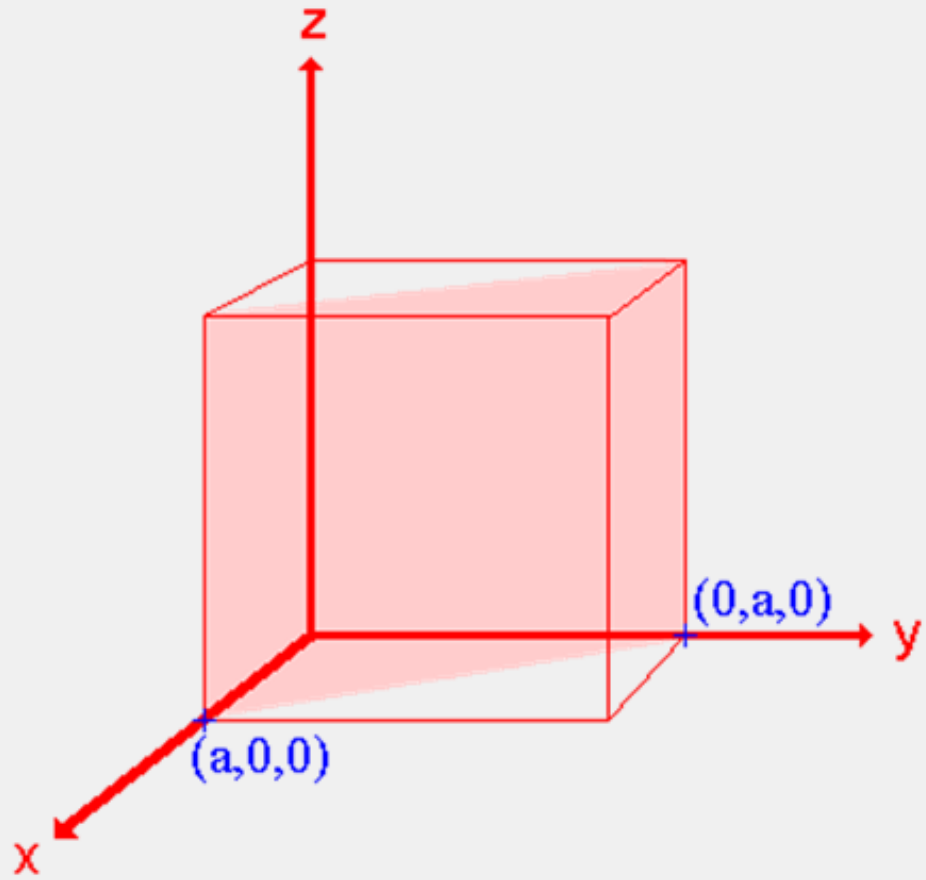


그림 3-26 여러 면의 밀러 지수 표시.

Other examples

1. The (110) surface



Assignment

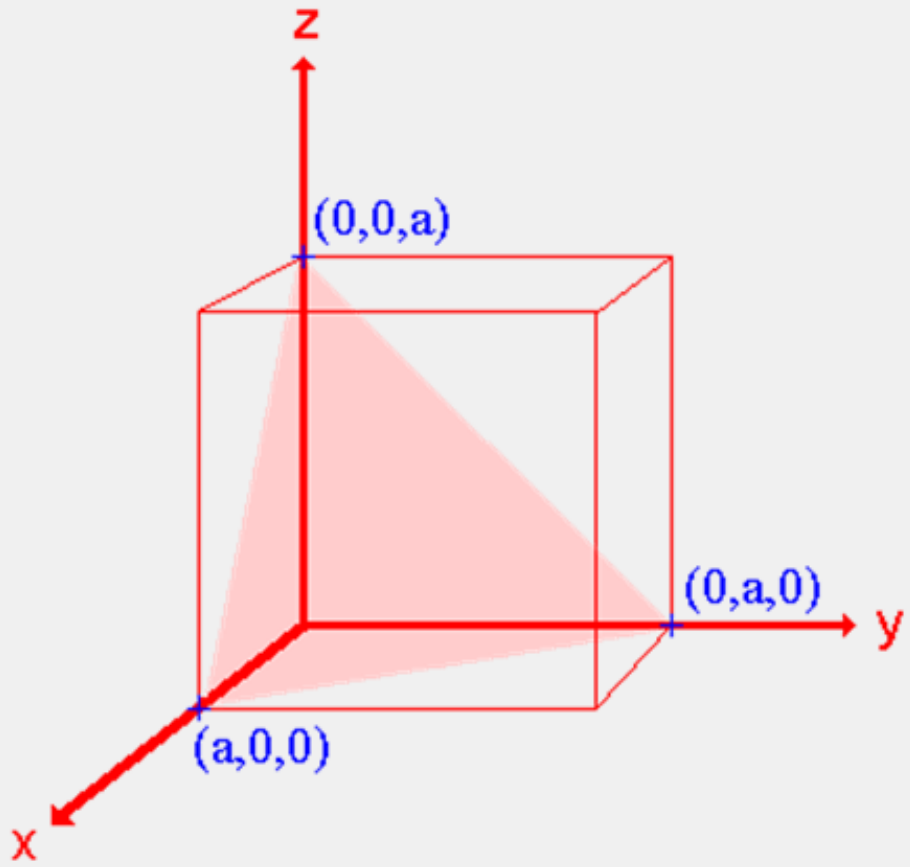
Intercepts : a , a , ∞

Fractional intercepts : 1 , 1 , ∞

Miller Indices : **(110)**

Other examples

2. The (111) surface



Assignment

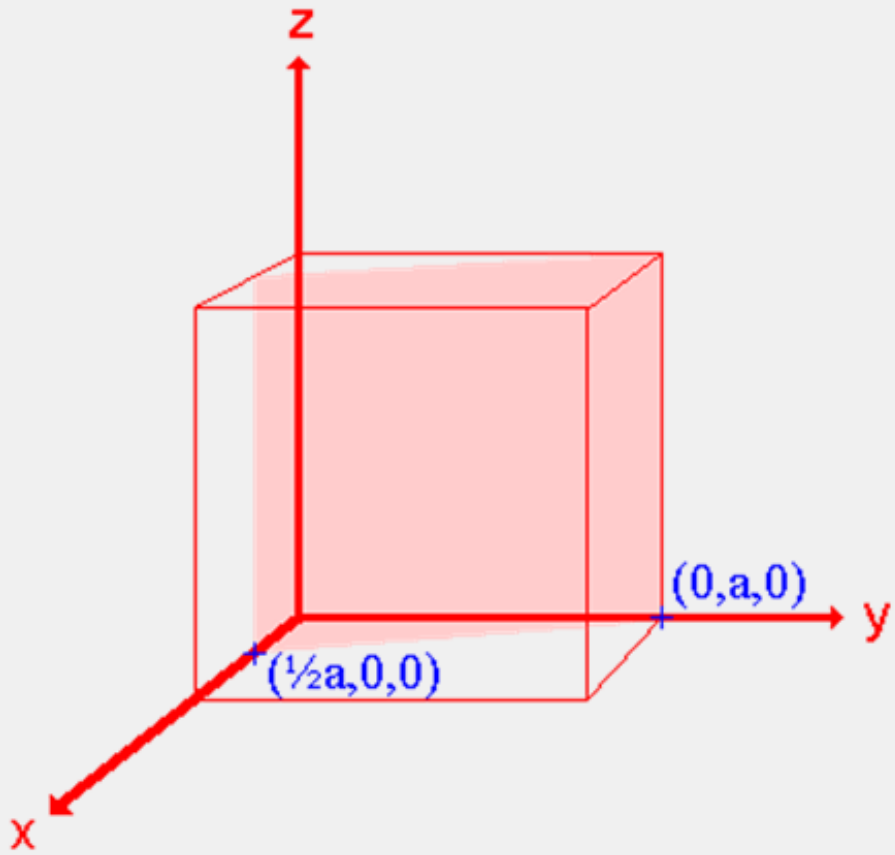
Intercepts : a , a , a

Fractional intercepts : 1 , 1 , 1

Miller Indices : **(111)**

Other examples

3. The (210) surface



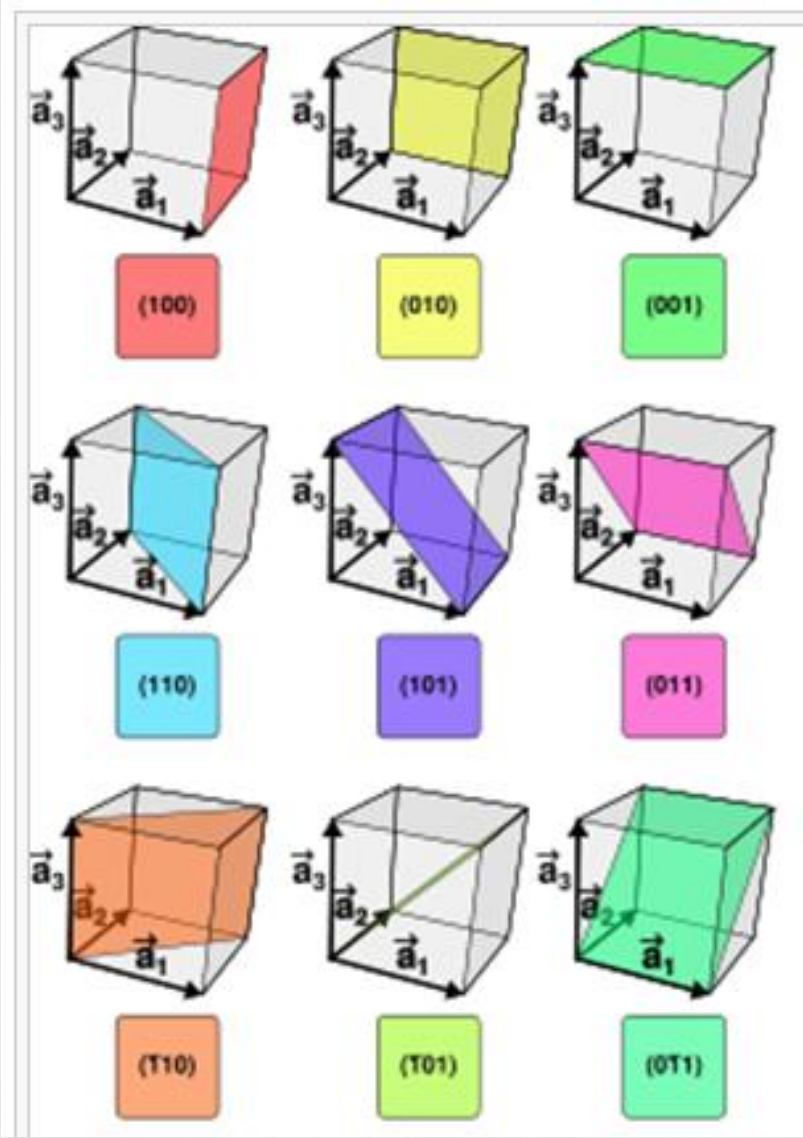
Assignment

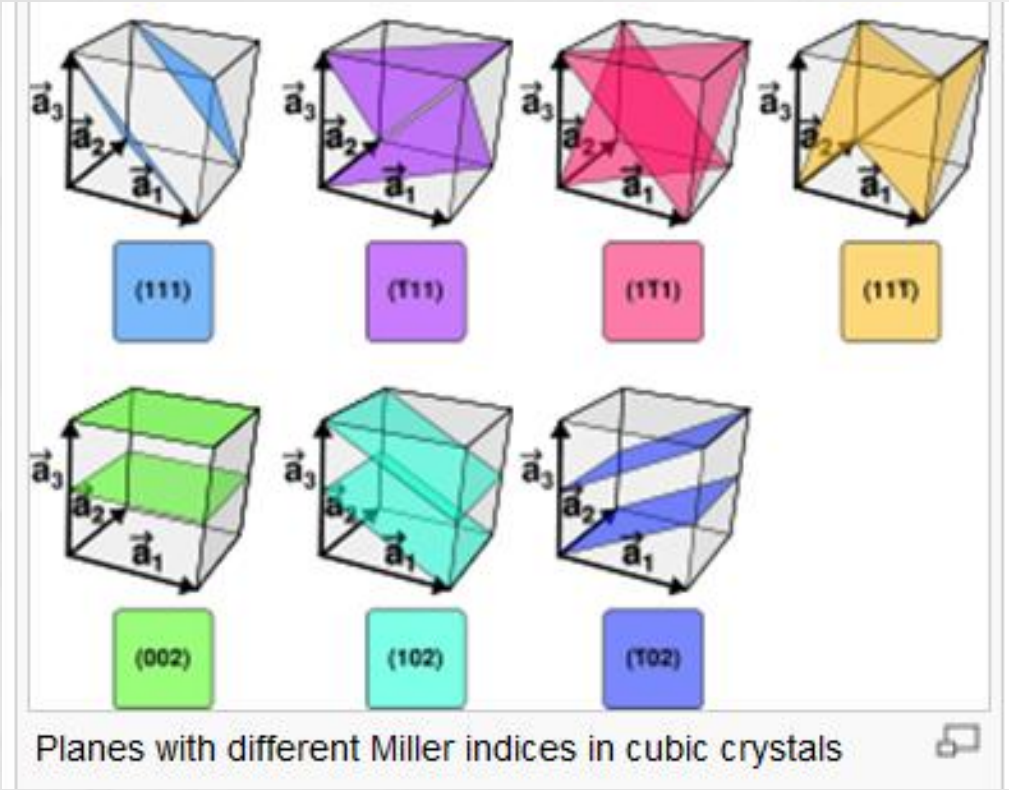
Intercepts : ½ *a* , *a* , ∞

Fractional intercepts : ½ , 1 , ∞

Miller Indices : **(210)**

Planes with different Miller Indices in cubic crystals





Applications of Miller index in crystals

- The equation of plane that has x, y and z intercepts at A, B and C, is given by

$$\frac{x}{A}+\frac{y}{B}+\frac{z}{C}=1 \qquad (3\text{-}19)$$

Where A=, B and C, is defined by $A = a/h', B = b/k', C = c/l'$

Then, the equation of plane will be expressed by

$$\frac{x}{a/h'}+\frac{y}{b/k'}+\frac{z}{c/l'}=1 \qquad (3\text{-}20)$$

Or

$$\frac{h'x}{a}+\frac{k'y}{b}+\frac{l'z}{c}=1 \qquad (3\text{-}21)$$

And, the equation of plane that is parallel to upper plane and pass through the origin will be given by

$$\frac{h'x}{a}+\frac{k'y}{b}+\frac{l'z}{c}=0 \qquad (3\text{-}22)$$

- If we remove the common factor of h', k', l' then we can get the equation of plane as following

$$\frac{hx}{a} + \frac{ky}{b} + \frac{lz}{c} = 0 \qquad (3\text{-}23)$$

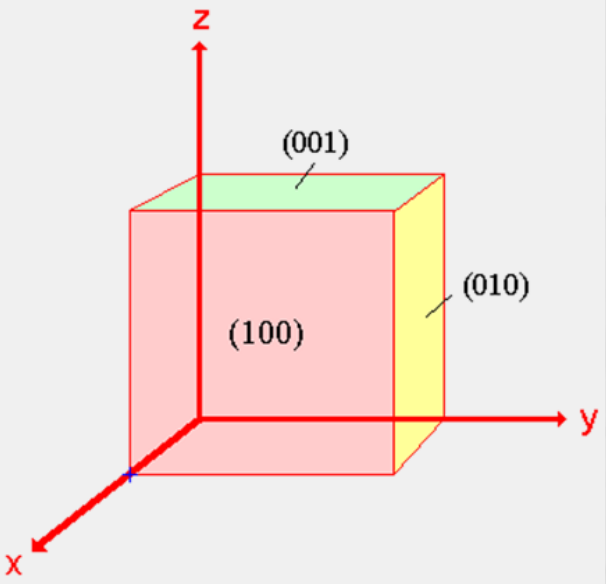
- Therefore, the equation for the total set of planes that are parallel to the upper plane can be given by

$$\frac{hx}{a} + \frac{ky}{b} + \frac{lz}{c} = m \qquad (3\text{-}24)$$

Where the (h k l) is the Miller index of the plane and *m* is integer

What are symmetry-equivalent surfaces ?

- In the following diagram the three highlighted surfaces are related by the symmetry elements of the cubic crystal - they are entirely equivalent.



- In fact there are a total of 6 faces related by the symmetry elements and equivalent to the (100) surface - any surface belonging to this set of symmetry related surfaces may be denoted by the more general notation {100} where the Miller indices of one of the surfaces is instead enclosed in curly-brackets.

Final important note *: in the cubic system the (hkl) plane and the vector [hkl], defined in the normal fashion with respect to the origin, are normal to one another* ***but*** *this characteristic is unique to the cubic crystal system and does* ***not*** *apply to crystal systems of lower symmetry.*

Miller-Bravais scheme for Hexagonal crystals

- If I am supposed to calculate the direction vector for the hexagonal crystal, I was told to:

  1) Calculate the line of projection of the vector (from origin to X) onto the base plane

  2) Calculate the new line of projection of this projected line with respect to a1 and a2 axis.

  3) Reduce the ratio of a1: a2 to the lowest integer

  4) Calculate the line of projection of the vector onto the verticle z axis

  5) Use the 3-index system to 4-index system formula to convert it and eventually get [11 (-2) 1] for the mentioned vector.

  However, this would imply that the z vector is independent of the ratio in a1 and a2 since using this method we would have gotten 0.5 unit length for a1 and a2 and 1 unit length for z. If not, shouldn't it be [11 (-2) 2] instead?

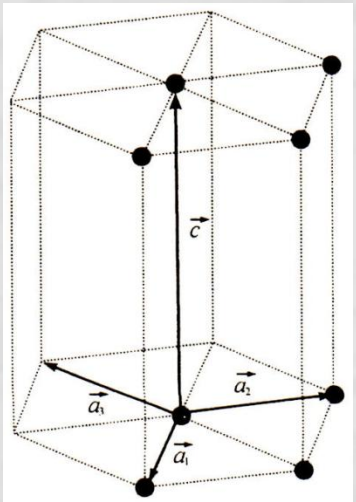
평면에서 2 개의 축으로 좌표를 표시할 수 있는데 3 개의 축을 사용하여 표시하였기 때문에 밀러-브라베 지수에서는 앞의 세 지수가 독립적이지 않다. 즉, $(h\ k\ i\ l)$에서 $h + k = -i$ 의 관계가 있다.

그림 3-27(b)는 면 $(h\ k\ i\ l)$이 a_1, a_2, a_3의 세 축이 있는 면과 만난 모습을 보여준다. 그림 3-27(b)에서 $OA = a_1/h$, $OB = a_2/k$, $OC = -a_3/i$ 이고 삼각형 OAB 의 면적은 두 삼각형 OAC 와 OCB 의 면적의 합이다. 그러므로,

$$\frac{1}{2}\frac{a_1}{h}\frac{a_2}{k}\sin 120^\circ = \frac{1}{2}\frac{a_1}{h}\frac{(-a_3)}{i}\sin 60^\circ + \frac{1}{2}\frac{(-a_3)}{i}\frac{a_2}{k}\sin 60^\circ$$

$$\frac{1}{hk} = \frac{-1}{hi} + \frac{-1}{ik} \qquad (3\text{-}25)$$

이 되어 $(h\ k\ i\ l)$에서 $h + k = -i$ 이다.



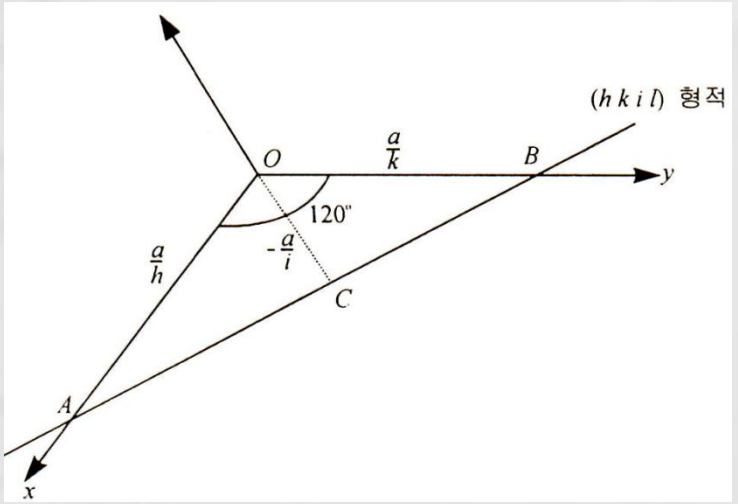


그림 3-27 (a) 밑면에 수직이면서 축 사이의 각도가 120°인 육방정 a_1, a_2, a_3, c 축, (b) 면 $(h\ k\ i\ l)$이 a_1, a_2, a_3의 세 축과 만나는 것을 나타낸다.