Lattice

Read

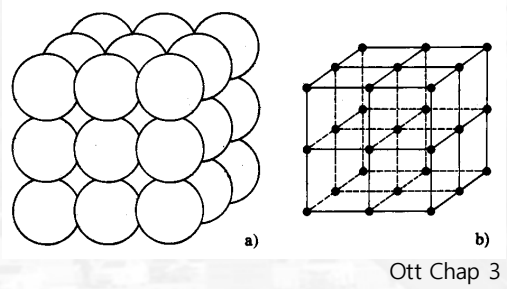
- Sherwood & Cooper 3.1 ~ 3.5
- Ott Chapter 3
- Hammond 2.1~2.5, 5.1~5.5
- Cullity 2.1; 2.2; 2.3
- Krawitz 1.3; 1.4

Lattice

- Lattice (격자) - an infinite array of points in space, where each point has **identical surroundings** to all others
- Crystal Structure (결정구조) - the 3-dimensional periodic arrangement of atoms in the crystal
- **Lattice + Motif (Basis) ⇒ Crystal structure**

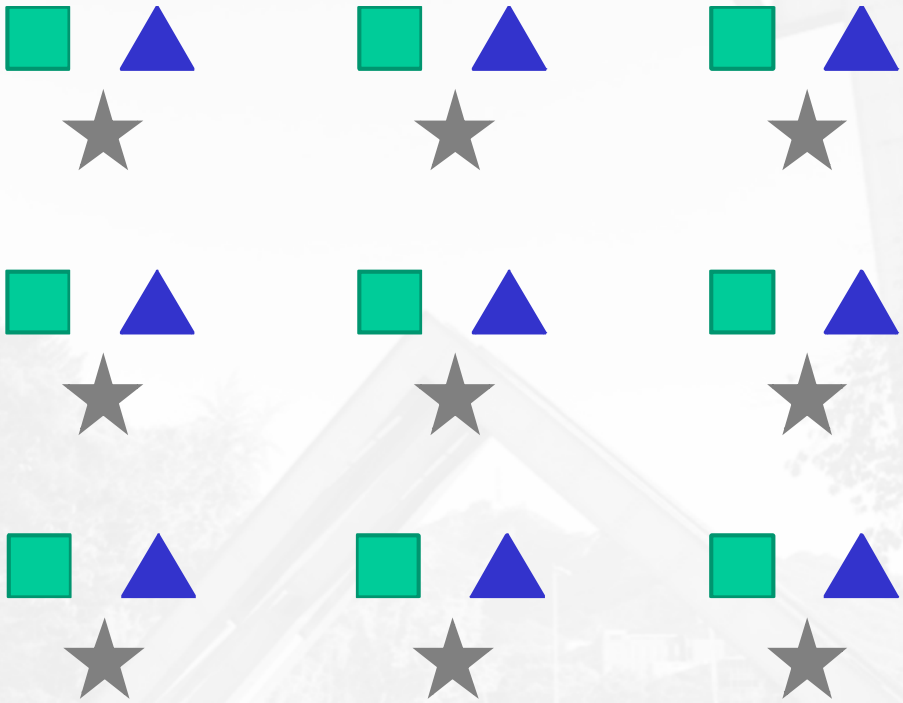
- each atom - its center of gravity - point or space lattice
- pure mathematical concept

α-polonium

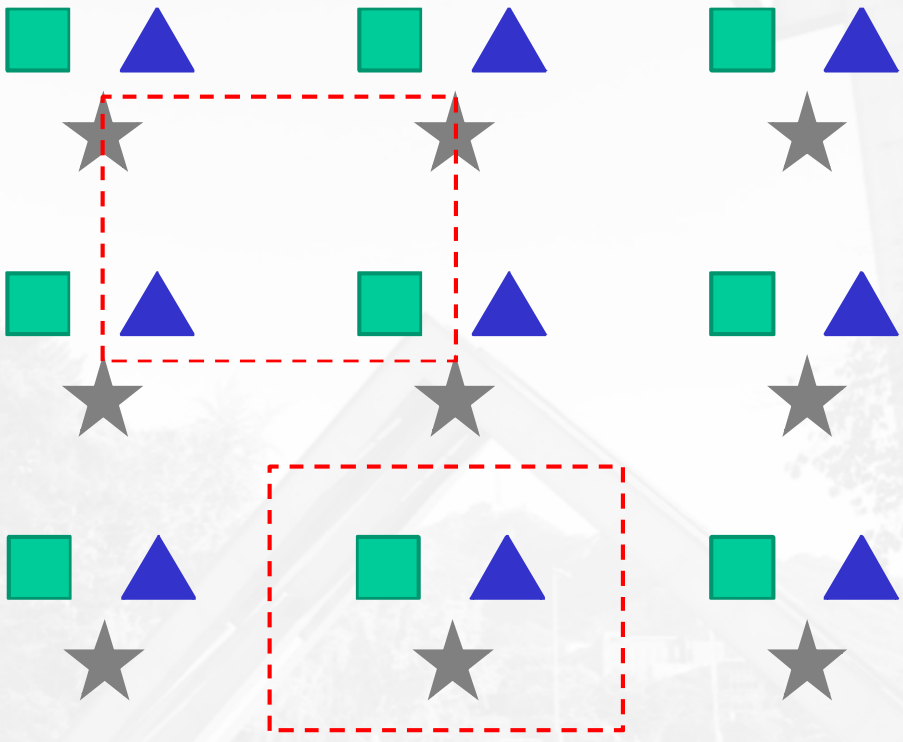


Ott Chap 3

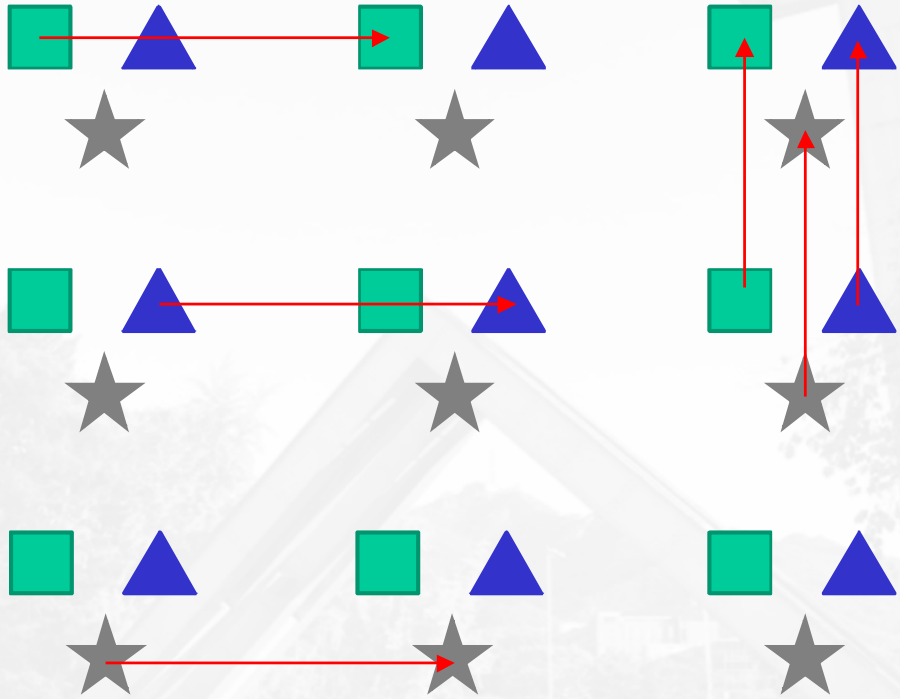
the smallest repeating unit = unit cell

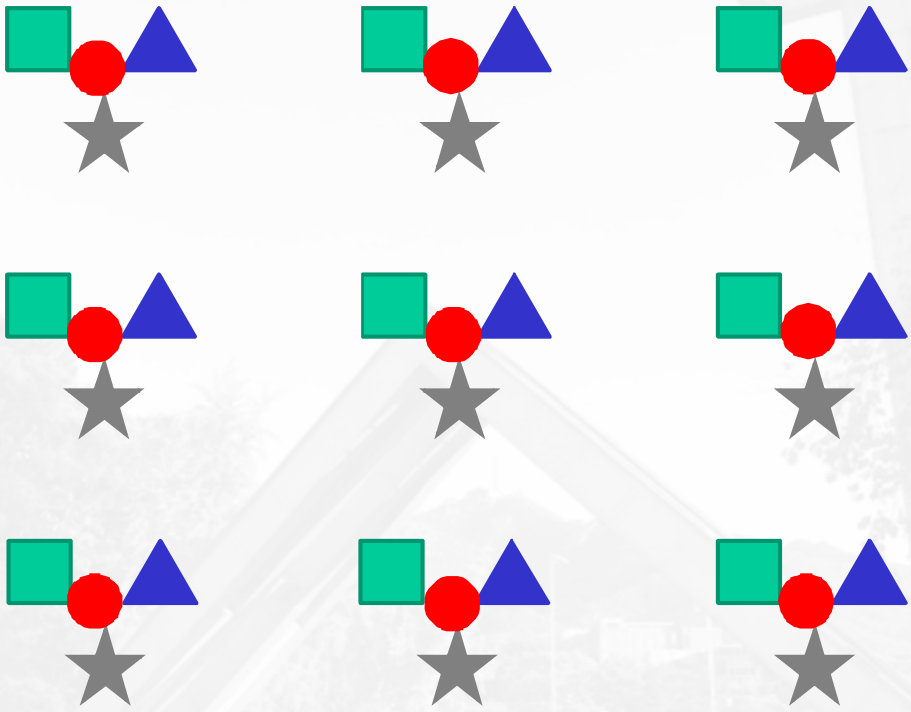


the smallest repeating unit = unit cell

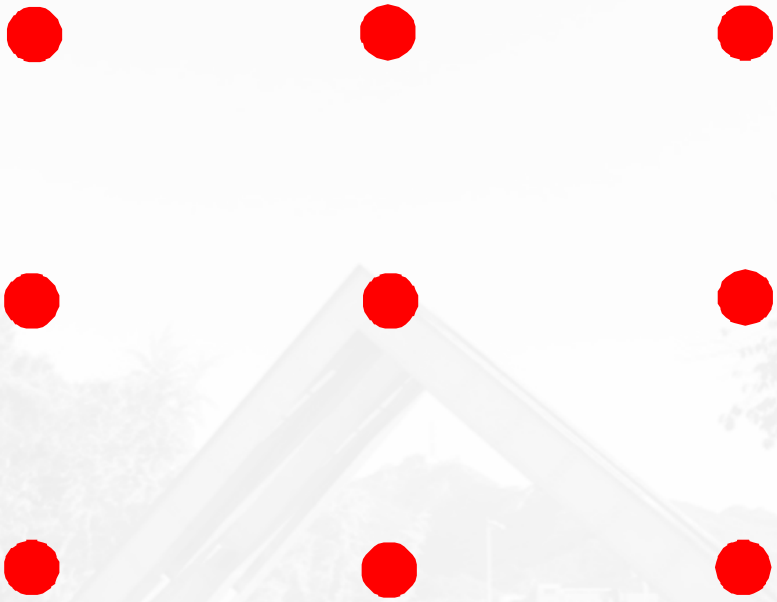


"Translation"



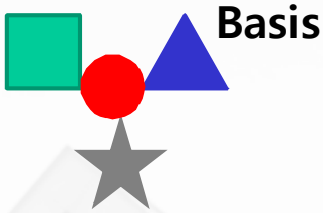


Lattice, lattice point



Lattice points: Identical surroundings

Basis

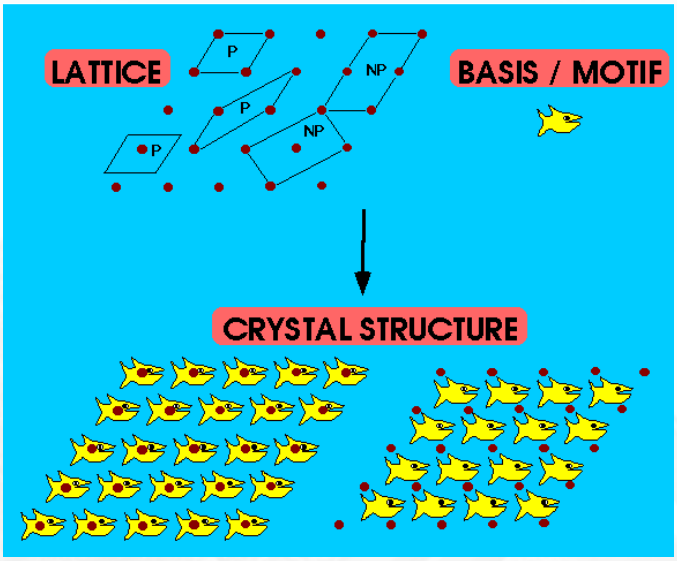


Lattice points: identical surroundings

Basis: patterns of atoms, molecule, ions

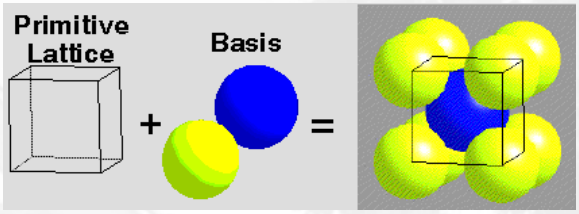
Crystal structure = lattice + basis

Lattice



Lattice + Motif (Basis)

→ Structure



➢What is the structure of the molecules within a crystal? → **motif**

➢What is the nature of the geometrical array which defines the way the molecules are arranged in space? → **lattice**

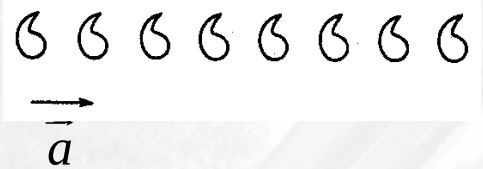
Lattice

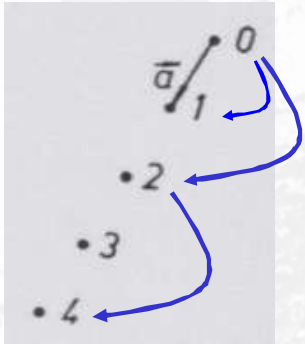
➢ lattice point → line lattice → plane lattice → space lattice

➢ Translation 0 → 1, 0 → 2, 2 → 4, etc.

This **repetition operation** → **Translation**

➢ Line lattice; A pattern produced by periodic repetition in one dimension and defined by translation $\vec{a}$,





line lattice

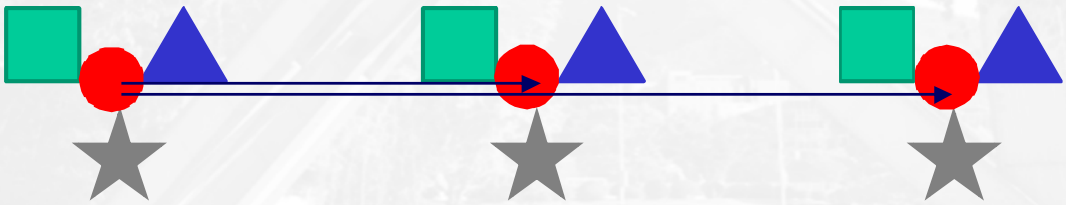
➢ Identical points (points equivalent by translation)

Line lattice

- A pattern produced by periodic repetition in one dimension and defined by translation vector $\vec{a}$ with lattice parameter (constant) *a*
- For any translation in 1-D

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

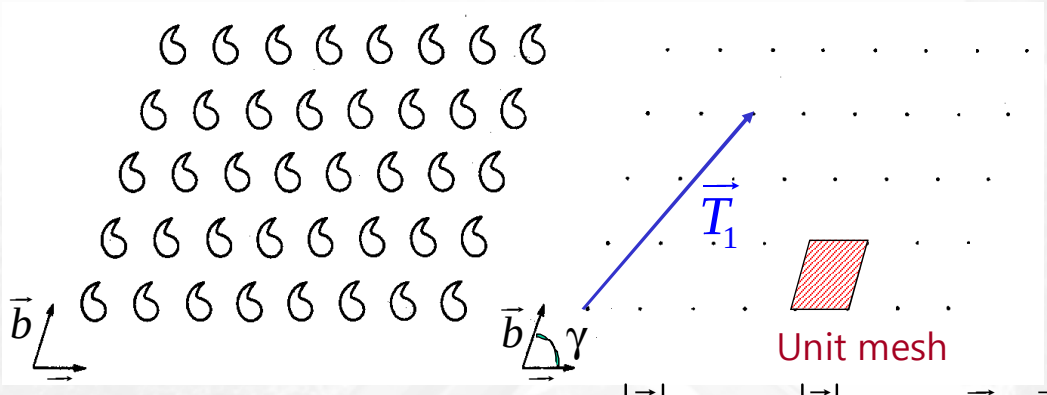
→ plane lattice, space lattice



Need just 1 vector to describe the line lattice.

Plane lattice

- A pattern produced by periodic repetition in two dimension and defined by translations in 2 directions.



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

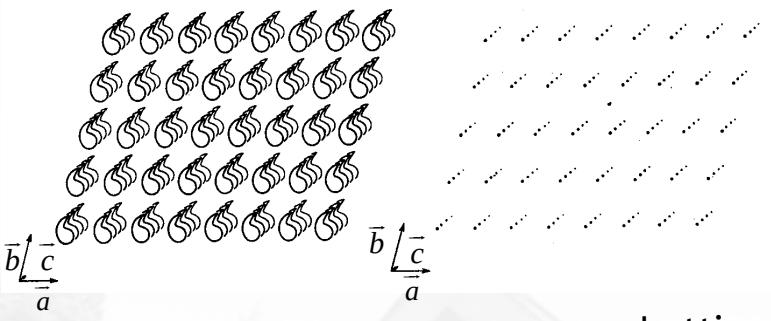
For any translation in 2-D, $\vec{T} = m\vec{a} + n\vec{b}$

$$-\infty < m < \infty, -\infty < n < \infty$$

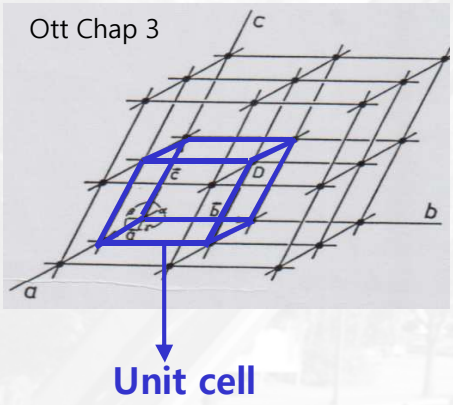
Need 2 vectors to describe the plane lattice.

Space lattice

- A pattern produced by periodic repetition in 3D and defined by translations in 3 directions.



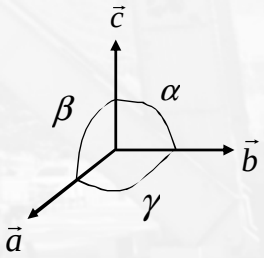
$$\vec{T} = m\vec{a} + n\vec{b} + p\vec{c}$$
$$-\infty < m < \infty$$
$$-\infty < n < \infty$$
$$-\infty < p < \infty$$



Lattice constants
Lattice parameters

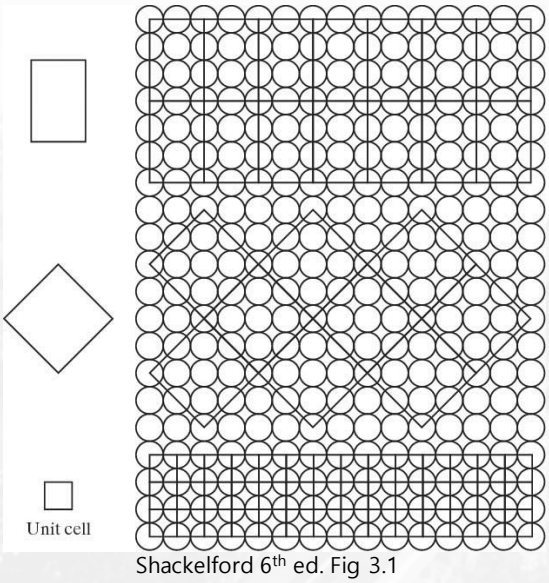
$$|\vec{a}| = a_0, \quad |\vec{b}| = b_0, \quad |\vec{c}| = c_0$$

$$\vec{a} \wedge \vec{b} = \gamma$$
$$\vec{a} \wedge \vec{c} = \beta$$
$$\vec{b} \wedge \vec{c} = \alpha$$



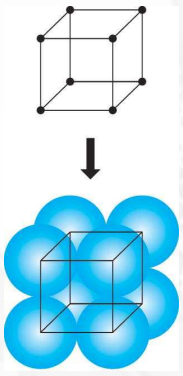
Unit cell

the smallest unit of volume that contains all of the structural and symmetry information and that can reproduce a pattern in all of space by translation.



Shackelford 6th ed. Fig 3.1

- The simple cubic lattice becomes the simple cubic crystal structure when an atom is placed on each lattice point



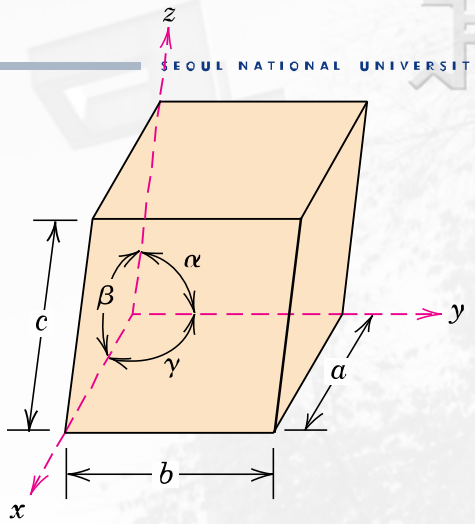
- Various structural units that describe the schematic crystalline structure
- The simplest structural unit → unit cell

An ASYMMETRIC UNIT
the smallest unit of volume that contains all of the structural information and that can reproduce the UNIT CELL by application of the symmetry operations.

Parameters to define a unit cell

Basis vectors : $\vec{a}$ $\vec{b}$ $\vec{c}$

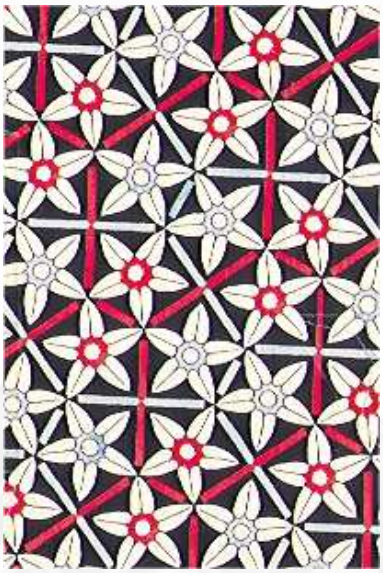
Lattice parameters : a b c α β γ

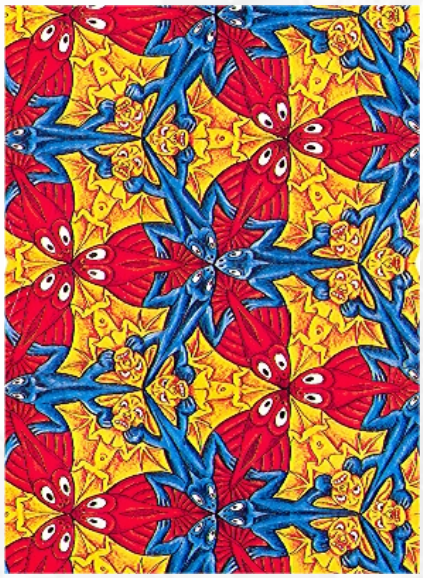


7 crystal systems

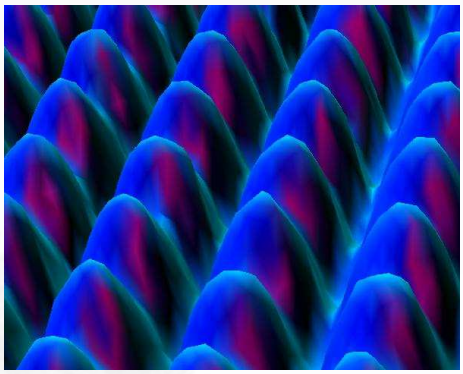
System	Conventional unit cell	
Triclinic	$\mathbf{a_1} \neq \mathbf{a_2} \neq \mathbf{a_3}$	$\alpha \neq \beta \neq \gamma$
Monoclinic	$\mathbf{a_1} \neq \mathbf{a_2} \neq \mathbf{a_3}$	$\alpha = \gamma, \quad \beta \geq 90°$
Orthorhombic	$\mathbf{a_1} \neq \mathbf{a_2} \neq \mathbf{a_3}$	$\alpha = \beta = \gamma = 90°$
Tetragonal	$\mathbf{a_1} = \mathbf{a_2} \neq \mathbf{a_3}$	$\alpha = \beta = \gamma = 90°$
Trigonal	$\mathbf{a_1} = \mathbf{a_2} = \mathbf{a_3}$	$\alpha = \beta = \gamma \neq 90°$
Hexagonal	$\mathbf{a_1} = \mathbf{a_2} \neq \mathbf{a_3}$	$\alpha = \beta = 90°, \gamma = 120°$
Cubic	$\mathbf{a_1} = \mathbf{a_2} = \mathbf{a_3}$	$\alpha = \beta = \gamma = 90°$

Unit cell

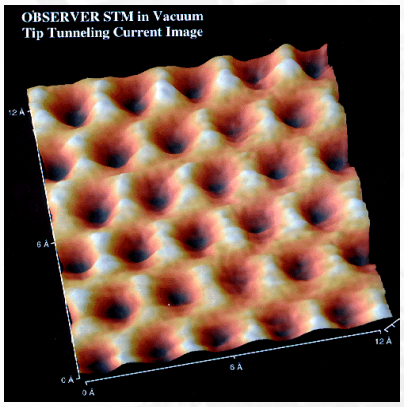




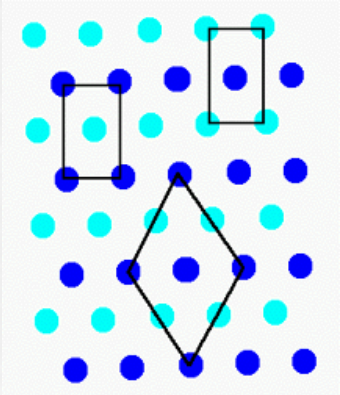
Lattice



STM image of Pt (IBM)

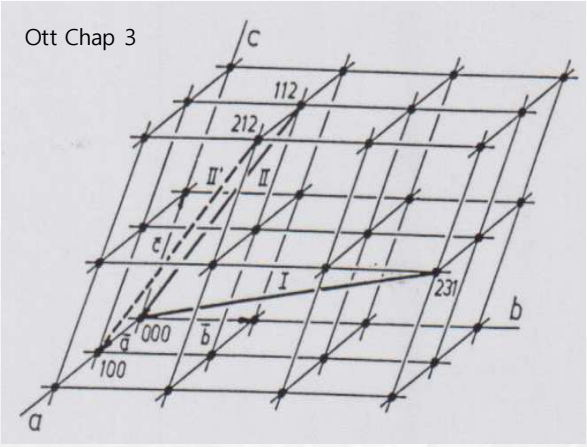


STM image of graphite



Selection of unit cell – simple, high symmetry

Lattice point, Lattice line



- Lattice Point **uvw**

  Every lattice point is uniquely defined with respect to the origin of lattice by vector .

  ex) 112, 212, 231

- Lattice Lines **[uvw]**

  Line : two points

  ex) I : 000 , 231 : [231]

  II : 000 , 112 : [112]

  II' : 100, 212 : [112]

[uvw]

(1) a lattice line through the origin and point uvw

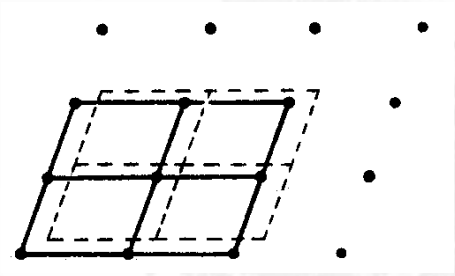
(2) the infinite set of lattice lines which are parallel to it and have the same lattice parameter

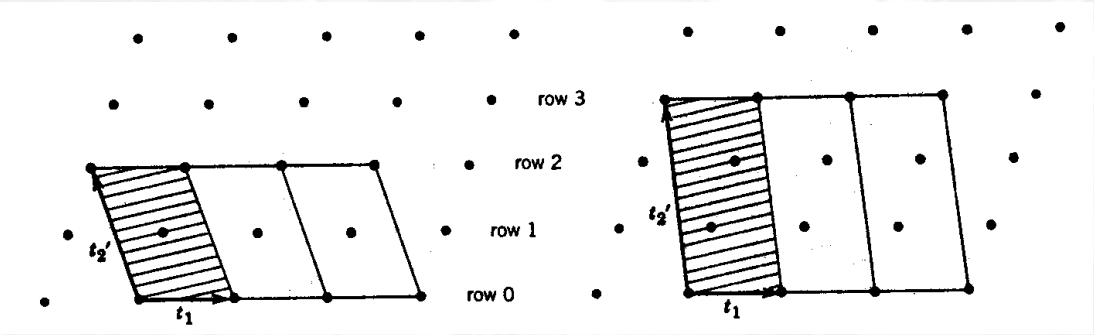
Primitive cell, non-primitive cell

For any translation

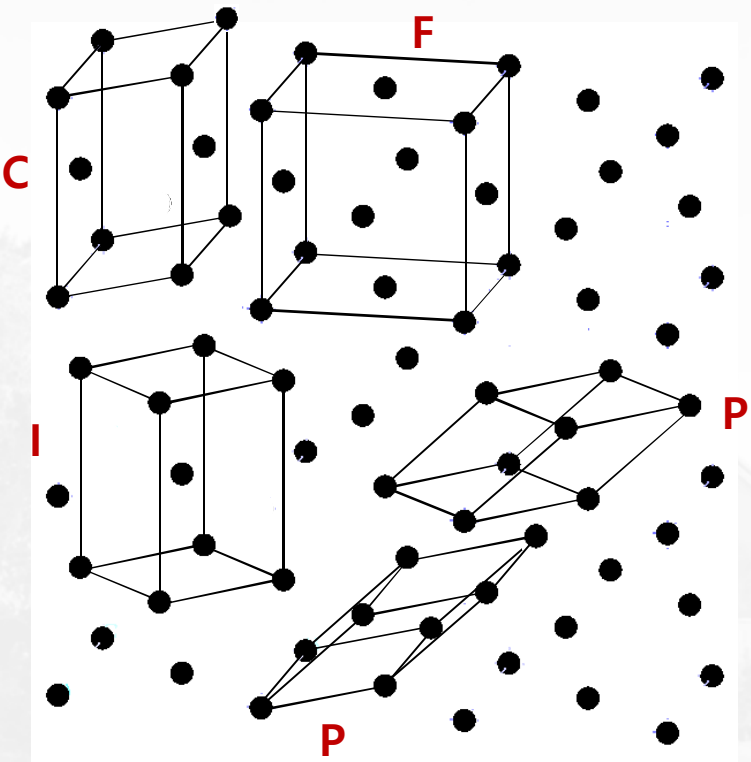
$$\vec{T} = m\vec{a} + n\vec{b} + p\vec{c} \qquad -\infty < m < \infty, -\infty < n < \infty, -\infty < p < \infty$$

- Primitive cell; one lattice point per cell
- Non-primitive cell; I, F, C, R

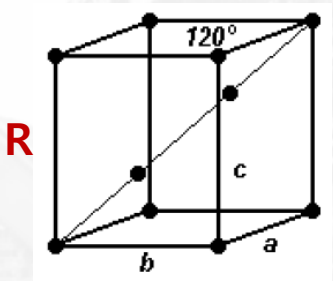




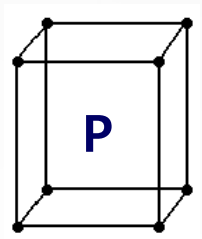
Lattice types - P, I, F, C, R



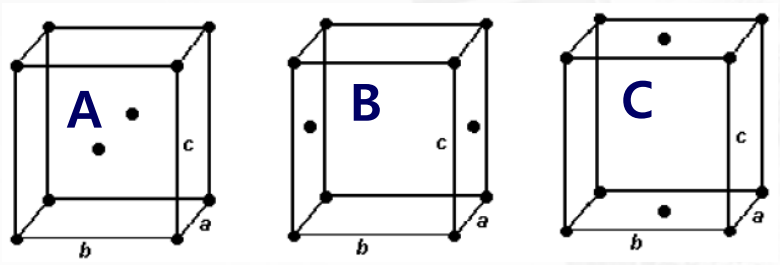
the number of lattice points in a unit cell?



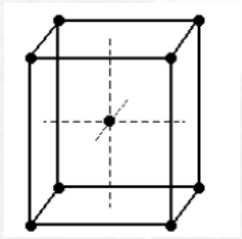
Lattice types - P, I, F, C, R



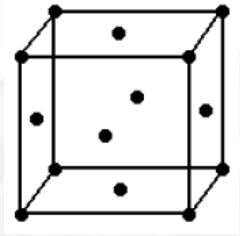
Primitive



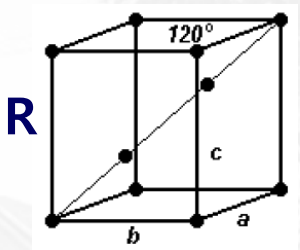
Base(end)-centered (C-centered)



- Body-centered
  - ✓ Point @ ½, ½, ½
  - ✓ Multiplicity = 2



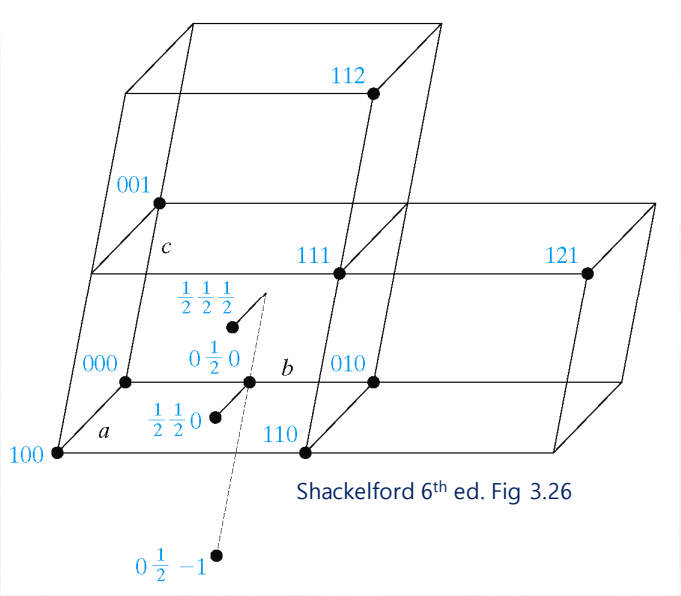
- Face-centered
  - ✓ ½, ½, 0
  - ✓ ½, 0, ½
  - ✓ 0, ½, ½
  - ✓ Multiplicity = 4



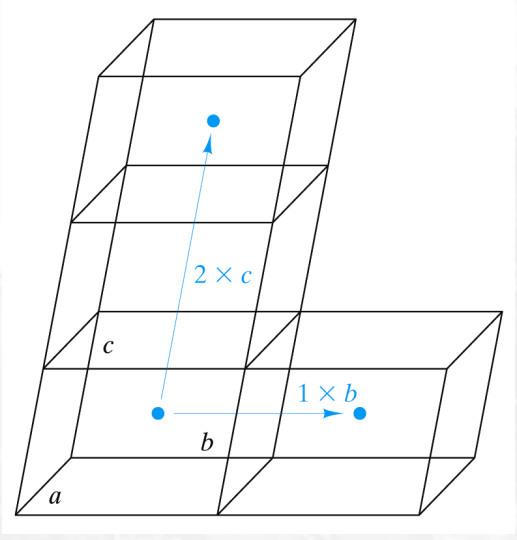
- Rhombohedral
  - ✓ 2/3, 1/3, 1/3
  - ✓ 1/3, 2/3, 2/3
  - ✓ Multiplicity = 3
  - ✓ Trigonal system

Lattice positions

Lattice translations connect structurally **equivalent** positions (e.g. the body center) in various unit cells



Shackelford 6th ed. Fig 3.26



Shackelford 6th ed. Fig 3.27

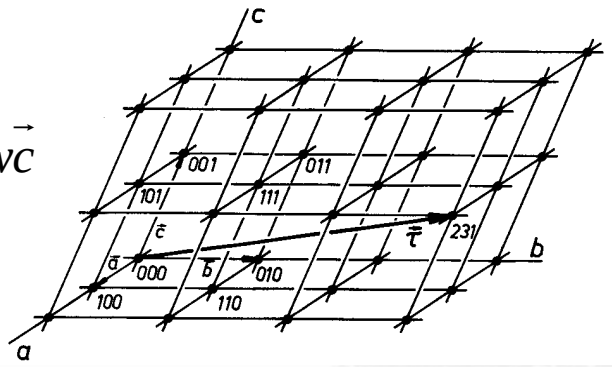
Lattice Point, Lattice Line

- 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

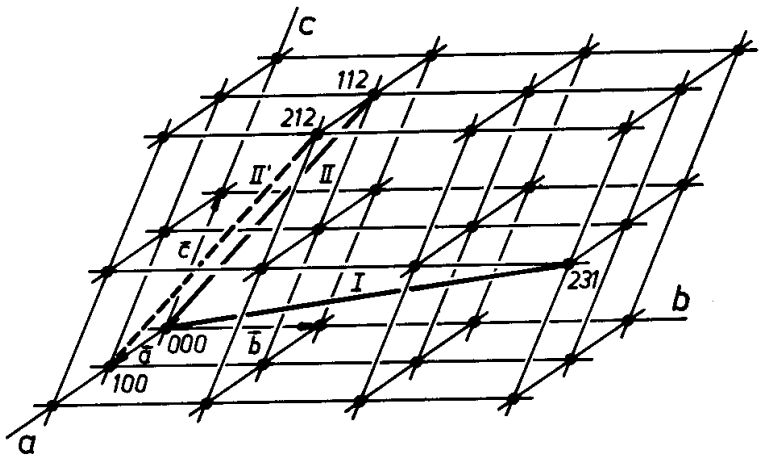
$\overline{u}\overline{v}\overline{w}$



- Lattice line [uvw]

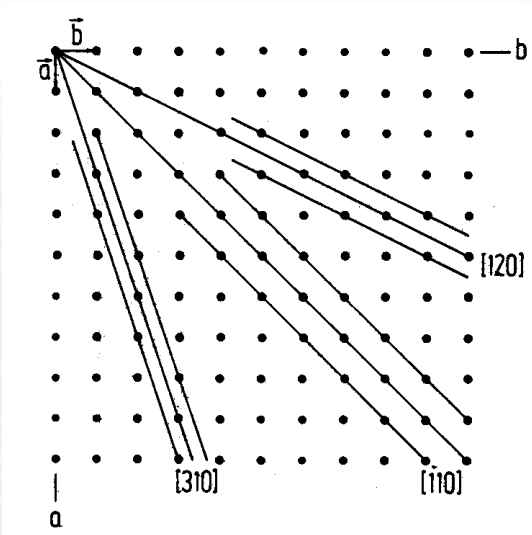
line - two points
I: 000 231 → [231]
II: 000 112 → [112]
II': 100 212 → [112]

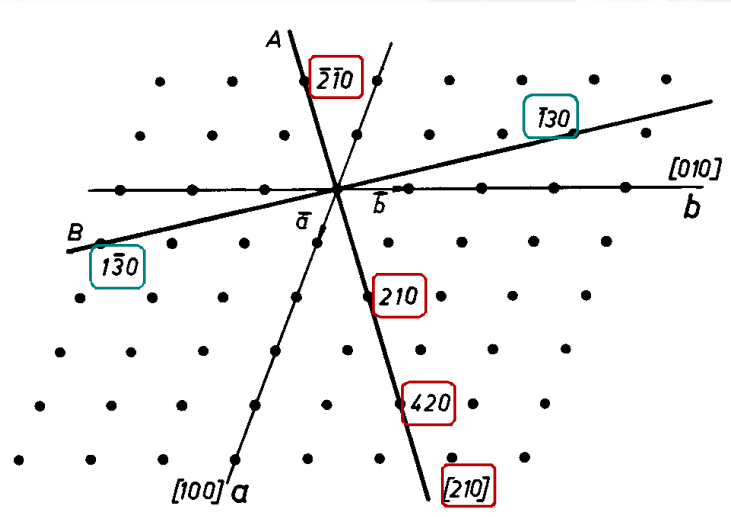
family <uvw>



[uvw]

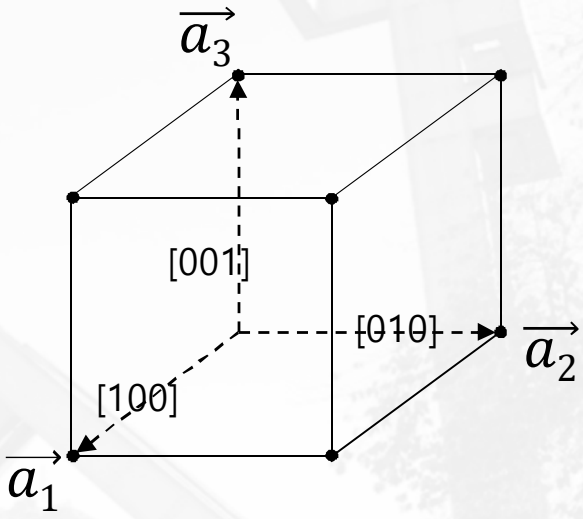
(1) a lattice line through the origin and point uvw
(2) the infinite set of lattice lines which are // to each other and have the same lattice parameter





- smallest integer 210, 420, $\bar{2}\bar{1}0$ → [210]
- opposite direction $\bar{1}30$ and $1\bar{3}0$

Equivalent Directions
= Family



cubic

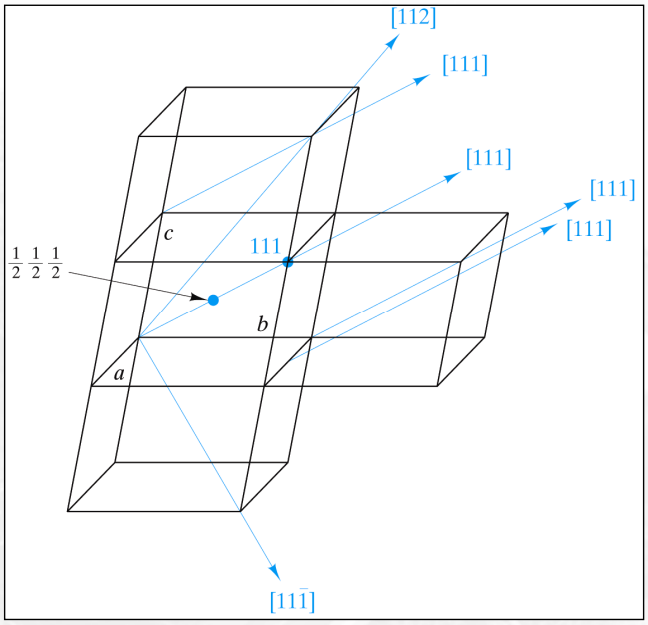
[1 0 0]	[0 1 0]	[0 0 1]
[$\bar{1}$ 0 0]	[0 $\bar{1}$ 0]	[0 0 $\bar{1}$]

< 1 0 0 >

Lattice directions

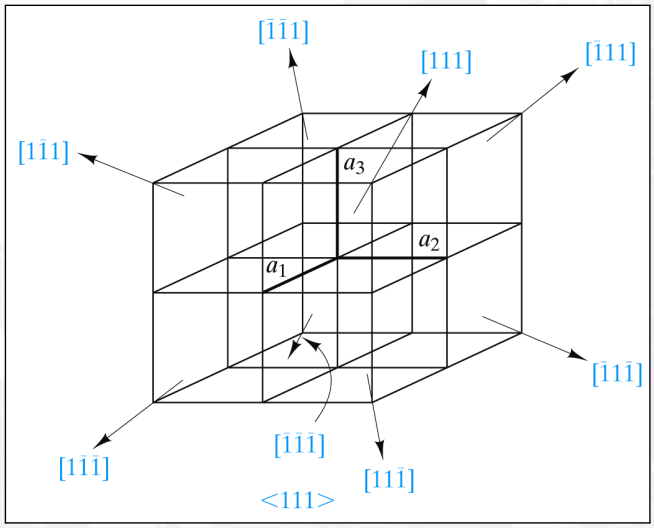
Family of directions

Parallel [uvw] directions share the same notation because only the origin is shifted



Shackelford 6th ed. Fig 3.28

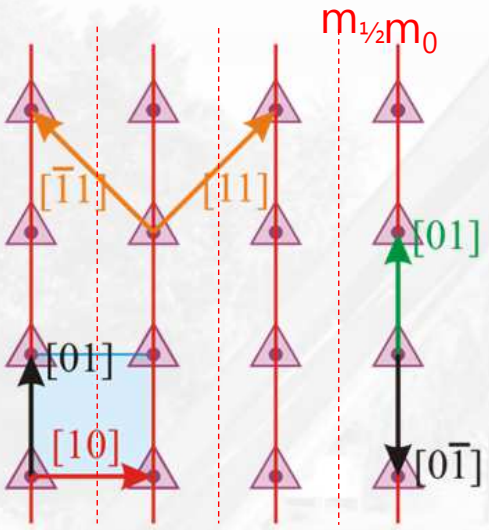
<111> represents all body diagonals

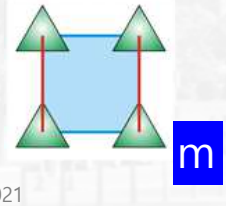


Shackelford 6th ed. Fig 3.29

Consider a square lattice decorated with a triangle to give a RECTANGLE CRYSTAL:

- [10] and [01] do NOT belong to the same family
  → 4-fold rotation destroyed in the crystal
- [11] and [$\bar{1}$ 1] belong to the same family → related by mirror
- [11] and [1 $\bar{1}$] do NOT belong to the same family
- [01] and [0 $\bar{1}$] do NOT belong to the same family





Writing down all the members of the family

$$<hk> \rightarrow [hk],[\bar{h}k]$$

$<10> \rightarrow [10],[\bar{1}0]$

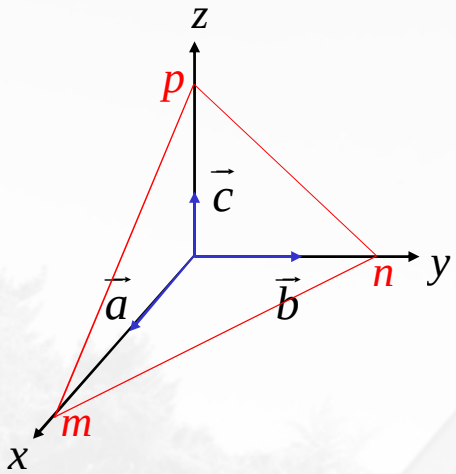
$<01> \rightarrow [01]$

$<0\bar{1}> \rightarrow [0\bar{1}]$

$<11> \rightarrow [11],[\bar{1}1]$

$<1\bar{1}> \rightarrow [1\bar{1}],[\bar{1}\bar{1}]$

Lattice plane (Miller index, Miller indices)



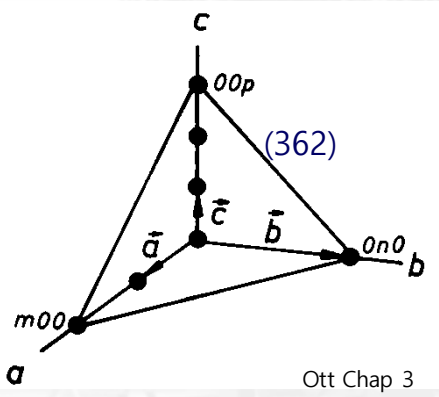
m00, 0n0, 00p: define a lattice plane

m, n, ∞ : no intercepts with c axis

Intercepts @ (mnp)	2	1	3
Reciprocals	½	1	1/3
Miller indicies	3	6	2
(362) plane			

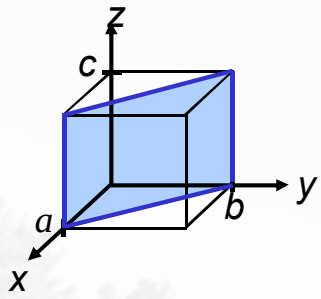
Plane (hkl)
Family of planes {hkl}

Miller indicies ; defined as the smallest integral multiples of the reciprocals of the plane intercepts on the axes

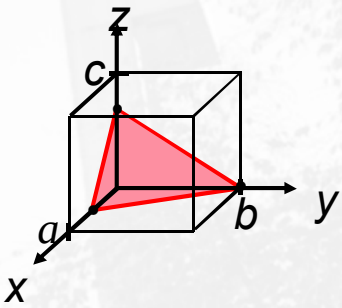


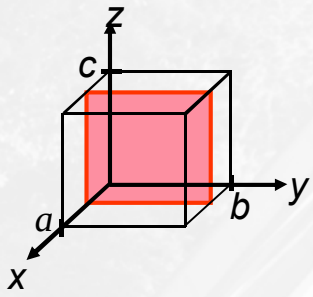
Ott Chap 3

Miller index



		a	*b*	*c*
①	Intercepts	1	1	∞
②	Reciprocals	1/1	1/1	1/∞
		1	1	0
③	Reduction	1	1	0
④	Miller Indices	(110)		

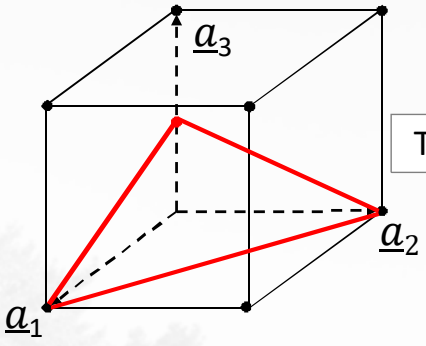




	a	*b*	*c*
①	1/2	∞	∞
②	1/½	1/∞	1/∞
	2	0	0
③	2	0	0
④	(200)		

	a	*b*	*c*
①	1/2	1	3/4
②	1/½	1/1	1/¾
	2	1	4/3
③	6	3	4
④	(634)		

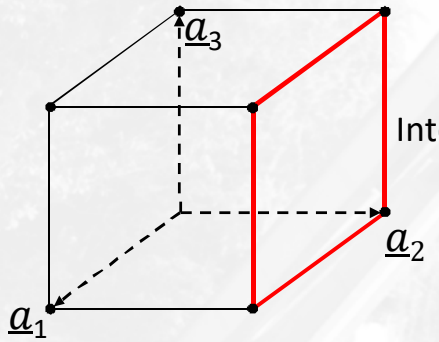
Miller index



Intercepts 1 1 $^1/_2$

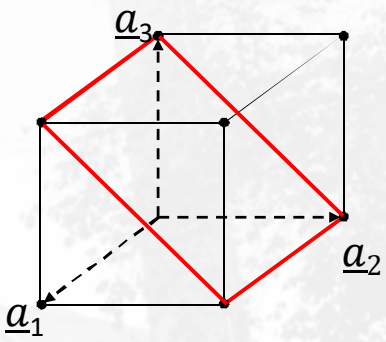
Take reciprocals and convert to integers

(1 1 2)



Intercepts ∞ 1 ∞

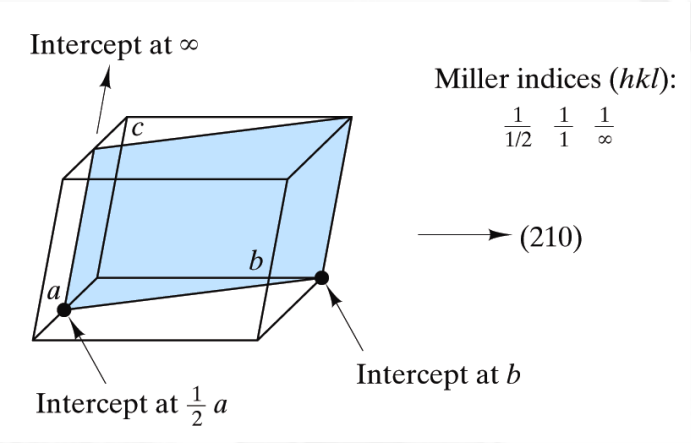
(0 1 0)

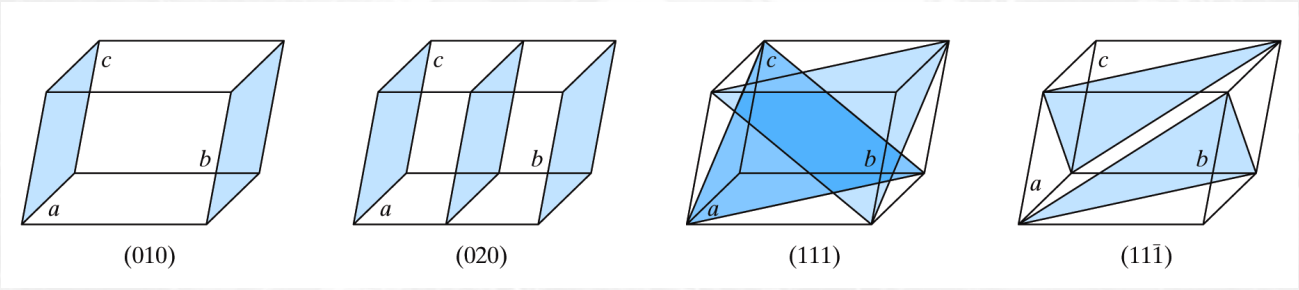


Intercepts ∞ 1 1

(0 1 1)

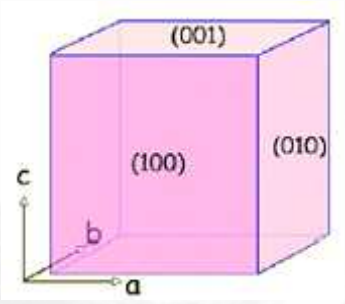
Lattice planes



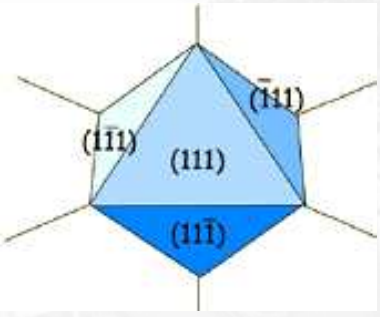


Lattice plane & crystal system

Crystal form: A set of equivalent faces is called a crystal form.
- There are approximately 48 unique crystal forms which are divided into either "open," "closed isometric," or "closed non-isometric" form categories.

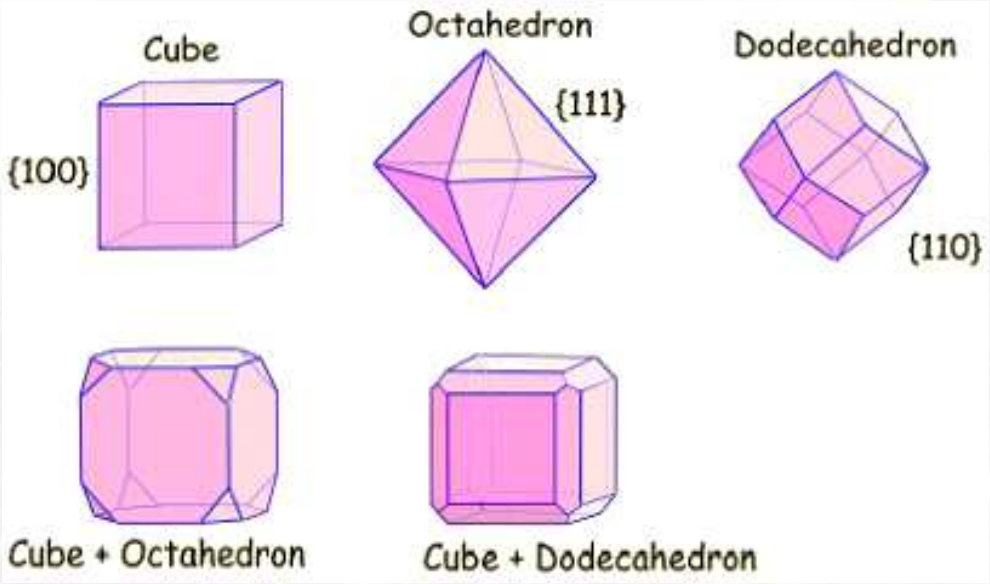


In a cubic system, {001} reproduces (001),(00$\bar{1}$), (010), (0$\bar{1}$0), (001), (00$\bar{1}$) and forms a cube resultantly.



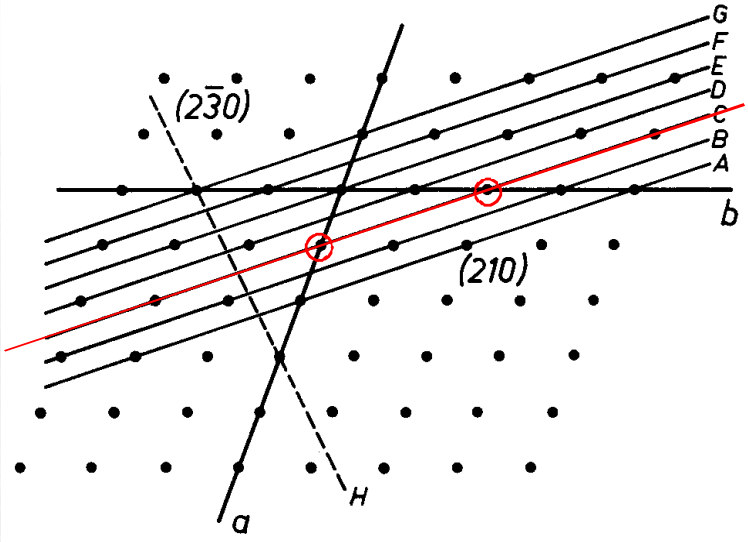
In a cubic system, {111} reproduces (111),($\bar{1}$11), (1$\bar{1}$1), (11$\bar{1}$), ($\bar{1}\bar{1}$1), ($\bar{1}$1$\bar{1}$), (1$\bar{1}\bar{1}$), ($\bar{1}\bar{1}\bar{1}$) and forms a octahedron resultantly.

Common cubic forms



Lattice plane (Miller indices)

(hkl) ; not merely a single plane, but **an infinite set of parallel planes with a constant interplanar spacing**



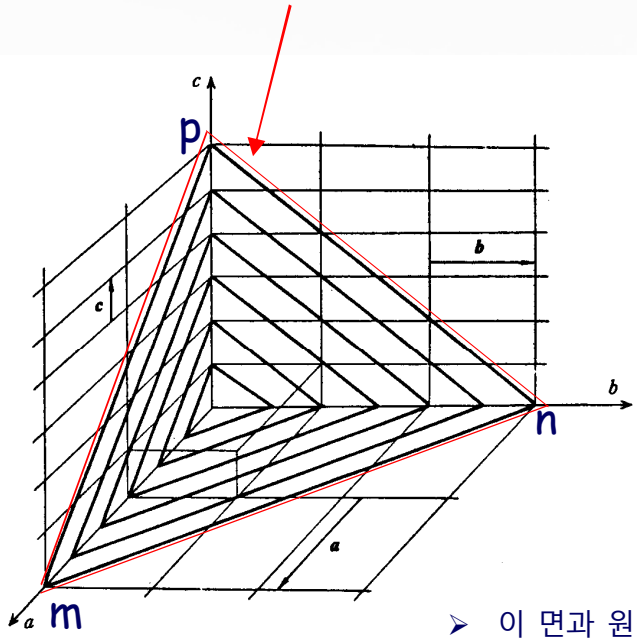
	m	n	p	$\frac{1}{m}$	$\frac{1}{n}$	$\frac{1}{p}$	(hkl)
A	2	4	∞	$\frac{1}{2}$	$\frac{1}{4}$	0	(210)
B	$\frac{3}{2}$	3	∞	$\frac{2}{3}$	$\frac{1}{3}$	0	(210)
C	1	2	∞	1	$\frac{1}{2}$	0	(210)
D	$\frac{1}{2}$	1	∞	2	1	0	(210)
E	–	–	–	–	–	–	
F	$\frac{\bar{1}}{2}$	$\bar{1}$	∞	$\bar{2}$	$\bar{1}$	0	($\bar{2}\bar{1}$0)
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 ↑, the spacing between the planes ↓, as does the density of points on each plane.

Ott Chap 3

Interplanar spacing d_{hkl}

- Rational intercept plane (유리교차면) - 세 축 상에서 모두 격자점과 교차하는 면



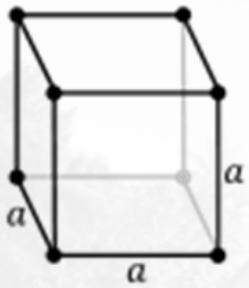
- intercept @ m, n, p
- m=2, n=3, p=6
- m, n의 최대공약수 r (2,3 →1)
- n, p의 최대공약수 s (3,6 → 3)
- p, m의 최대공약수 t (2,6 → 2)

Intercepts @ (mnp)	2	3	6
Reciprocals	½	1/3	1/6
Miller indicies	3	2	1
(321) plane			

- 이 면과 원점 사이에는 mnp/rst (36/6 = 6) 개의 면이 있다
- 이 때 각 면들간의 거리를 d_{hkl} 이라 한다
- np/rst=3 (h), pm/rst=2 (k), mn/rst=1 (l)

Planes of a form or a family of planes
: sets of equivalent lattice planes related by symmetry

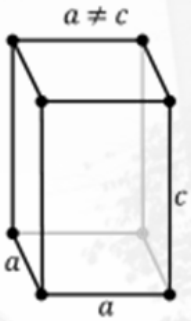
Cubic



{100} : (100), ($\bar{1}$00), (010)
(0$\bar{1}$0), (001), (00$\bar{1}$)

A 4-fold rotation axes ⊥ to all the cube faces

Tetragonal

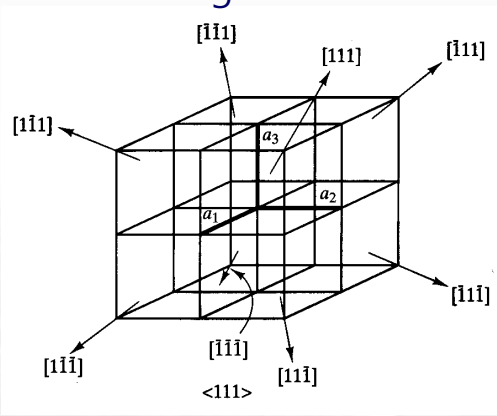


{100} : (100), ($\bar{1}$00), (010), (0$\bar{1}$0)
{001} : (001), (00$\bar{1}$)

A 4-fold axis for the first four planes
A 2-fold axis for the last two

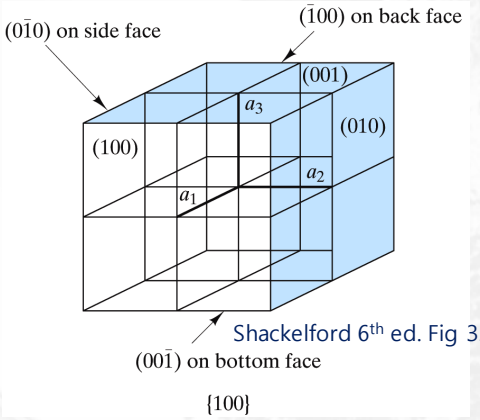
Family of directions and planes

Family of lines
<111> angular bracket



[111] square bracket
line, direction

Family of planes
{100} braces



Shackelford 6th ed. Fig 3.32

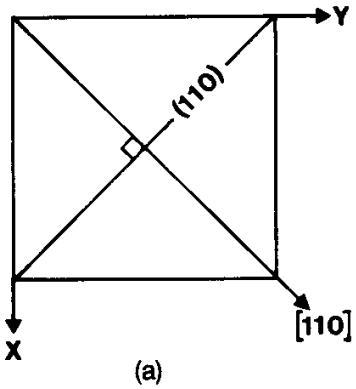
(100) round bracket
(parentheses)
plane

{100} of cubic = (100), (010), (001), ($\bar{1}$00), (0$\bar{1}$0), (00$\bar{1}$)

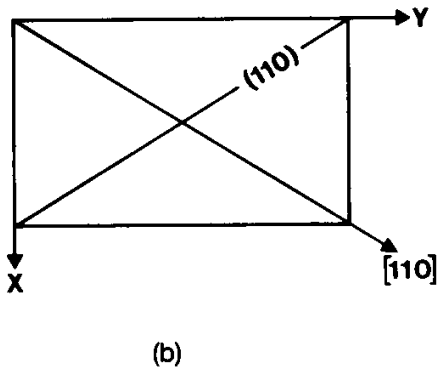
{100} represents all faces of unit cells in the cubic system

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.

Hammond Fig 5.5

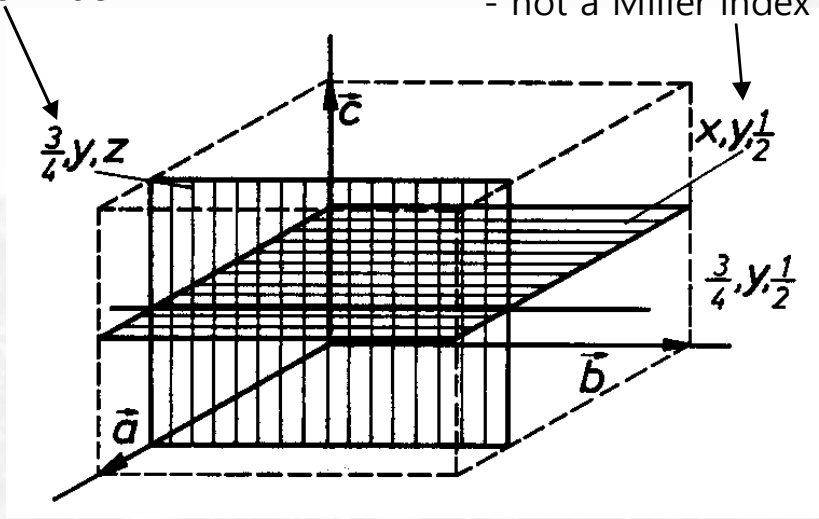
See Sherwood & Cooper Chap 3.5

Hammond Chap 5

Planes and Lines in the cell

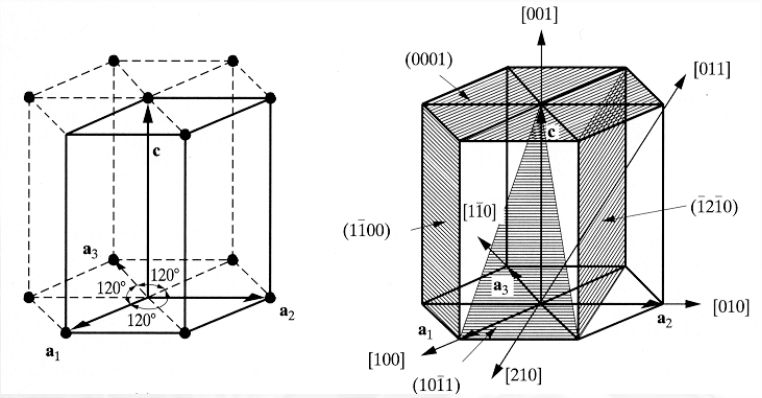
- all points in the plane // to b and c axes which cuts a axis @ ¾
- not a Miller index

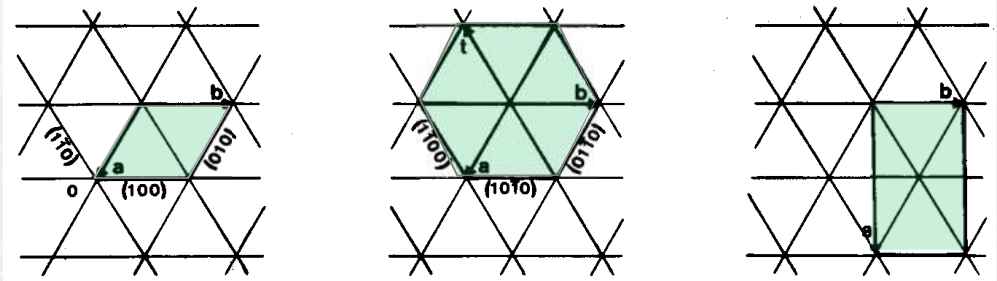
- all points in the plane // to a and b axes which cuts c axis @ ½
- not a Miller index



Unit cell of hexagonal

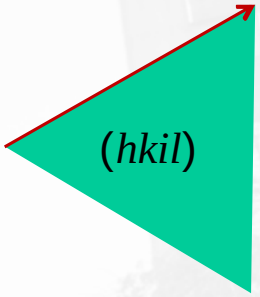
- hexagonal coordinate a_1, a_2, a_3, c
- Miller-Bravais indices (h k i l) i = - (h+k)



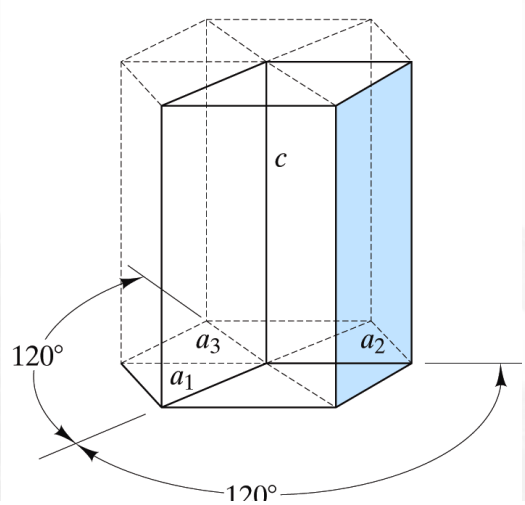


Miller Bravais index (hkil) for hexagonal system

[*uvtw*]



$hu + kw + iv + lw \neq 0$ in Miller-Bravais indices.

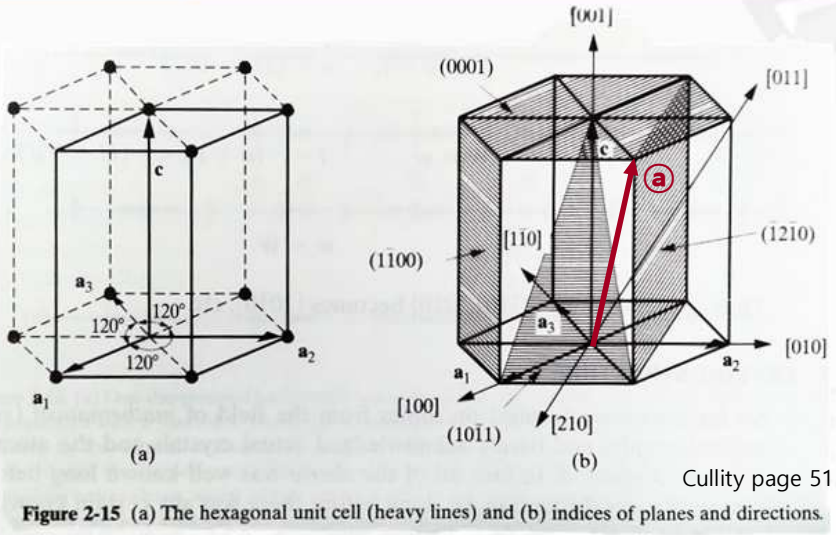


Miller–Bravais indices $(hkil)$: $\frac{1}{\infty}, \frac{1}{1}, \frac{1}{-1}, \frac{1}{\infty} \rightarrow (01\bar{1}0)$

Note: $h + k = -i$

Shackelford 6th ed. Fig 3.31

[*uvw*] → [*UVTW*]



ⓐ: [????]

Cullity page 51

Figure 2-15 (a) The hexagonal unit cell (heavy lines) and (b) indices of planes and directions.

$u = U - T$
$v = V - T$
$w = W$

$U = (2u - v)/3$
$V = (2v - u)/3$
$T = -(u + v)/3$
$W = w$

[100] becomes [2$\bar{1}\bar{1}$0]

[210] becomes [10$\bar{1}$0]

Hammond chap 5.7

Weiss zone law, zonal equation

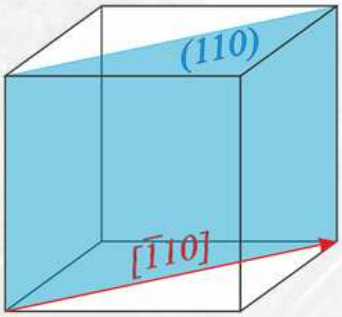
- If the Miller plane **(hkl)** contains *(or is parallel to)* the direction **[uvw]** then:

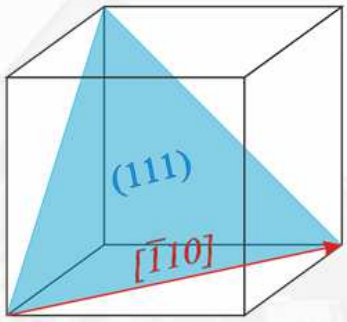
$$h.u + k.v + l.w = 0$$ Zonal equation

- This relation is valid for all crystal systems *(referring to the standard unit cell).*

The red directions lie on the blue planes.

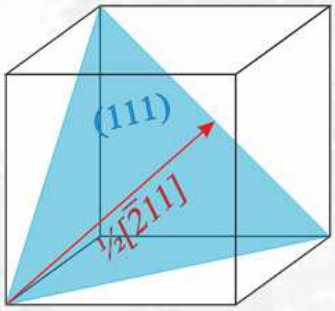
$$(1\cdot\bar{1})+(1\cdot 1)+(0\cdot 0)=0$$





$$(1\cdot\bar{1})+(1\cdot 1)+(1\cdot 0)=0$$

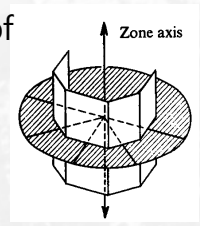
$$\tfrac{1}{2}\left[(1\cdot\bar{2})+(1\cdot 1)+(1\cdot 1)\right]=0$$



Hammond chapter 5.6
Ott chap 3.5

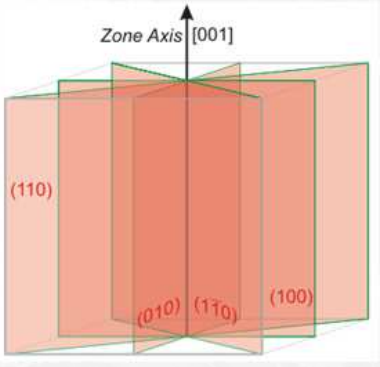
Zone, zone axis

- Zone ; a set of non-// planes which are all // to one axis (called zone axis)
- Zone ; a set of planes whose intersections are all //.
- Zone axis [*uvw*]; the common direction of the intersection of a set of planes in a zone
- Miller indices (hkl) for all planes in a zone follow $hu + kv + lw = 0$
- Example – pencil



- The direction common to a set of planes is called the zone axis of those planes.
- If $(h_1\ k_1\ l_1)$ & $(h_2\ k_2\ l_2)$ are two planes having a common direction [uvw] → according to Weiss zone law:

$uh_1 + vk_1 + wl_1 = 0$ & $uh_2 + vk_2 + wl_2 = 0$



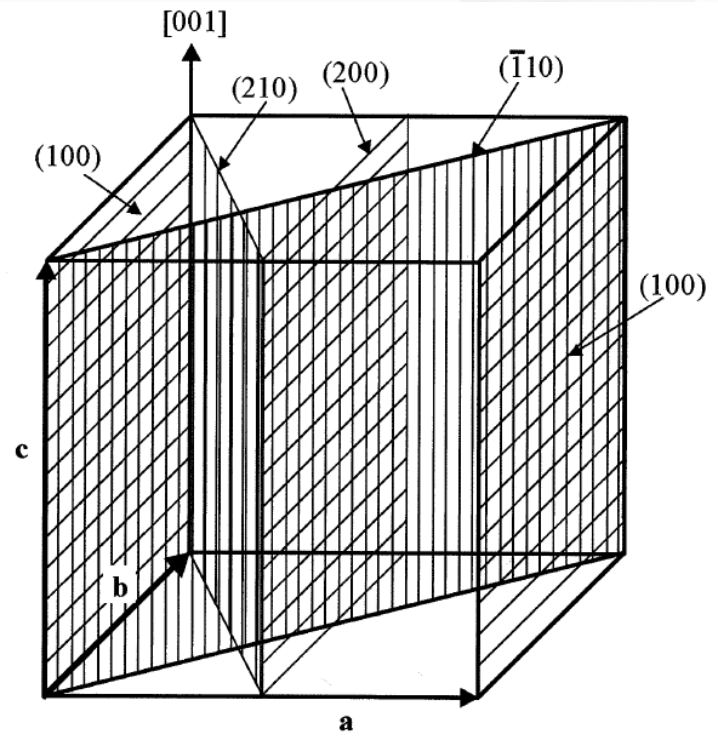
[001] lies on (110), (1$\bar{1}$0), (010), (100)

ideas.ted.com/quiz-how-much-do-you-really-know-about-the-pencil/

Hammond chapter 5.1; 5.6
Ott chap 3.5

Zone, zone axis

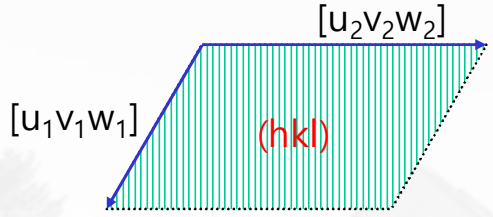
Planes belonging to [001] zone in cubic lattice



Zonal equation

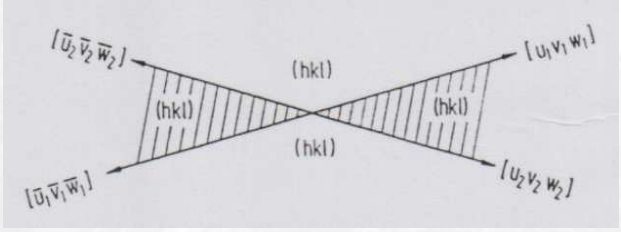
- Two lattice lines $[u_1v_1w_1]$ and $[u_2v_2w_2]$ lie in the lattice plane (hkl). (hkl) can be determined from the zonal equation.

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



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

- Two non-parallel lattice lines determine a lattice plane



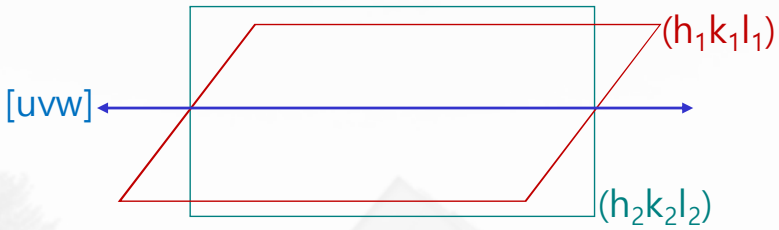
$$h:k:l = \begin{vmatrix} v_1 & w_1 \\ v_2 & w_2 \end{vmatrix} : \begin{vmatrix} w_1 & u_1 \\ w_2 & u_2 \end{vmatrix} : \begin{vmatrix} u_1 & v_1 \\ u_2 & v_2 \end{vmatrix}$$

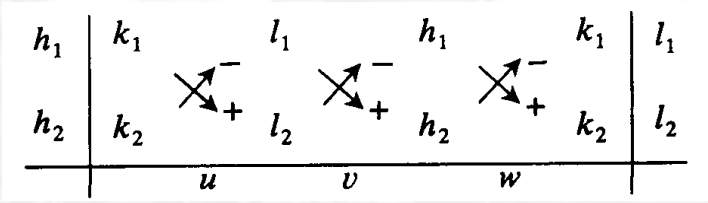
Ott page 17

Hammond chapter 5.1; 5.6
Ott chap 3.5

- Two lattice planes $(h_1k_1l_1)$ and $(h_2k_2l_2)$ intersect in the lattice line [uvw]

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





$u = (k_1l_2 - k_2l_1)$; $v = (l_1h_2 - l_2h_1)$; $w = (h_1k_2 - h_2k_1)$

Hammond chapter 5.1; 5.6
Ott chap 3.5

todos

- Tons of info in internet including "www.iucr.org/education"

- Read
  - Sherwood & Cooper 3.1 ~ 3.5
  - Ott Chapter 3, 4
  - Hammond 2.1~2.5, 5.1~5.5
  - Cullity 2.1; 2.2; 2.3
  - Krawitz 1.3; 1.4

- Lattice Homework (due in 1 week)
  - ✓ Ott Chapter 3 --- problem 2, 3, 4, 5, 6
  - ✓ Cullity chapter 2 --- 1, 2, 3, 5, 6