

2019 Fall

Introduction to Materials Science and Engineering

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Contents for previous class

Atomic Bonding in Solids : an attempt to fill electron shells

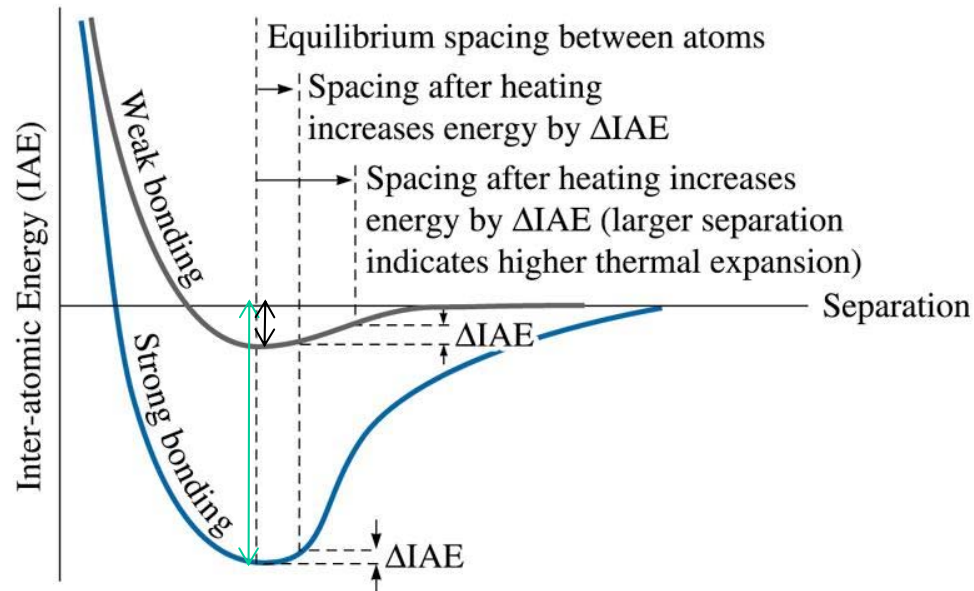
a. Primary bonding

- (1) Ionic bonds
- (2) Covalent bonds
- (3) Metallic bonds

b. Secondary bonding

- (1) Van der Waals
- (2) Hydrogen bonding

c. Properties From Bonding



If E_0 is larger,

T_m (melting temp. \rightarrow Broken Bonds),

E (elastic modulus), ((possibly))

Yield strength is larger,

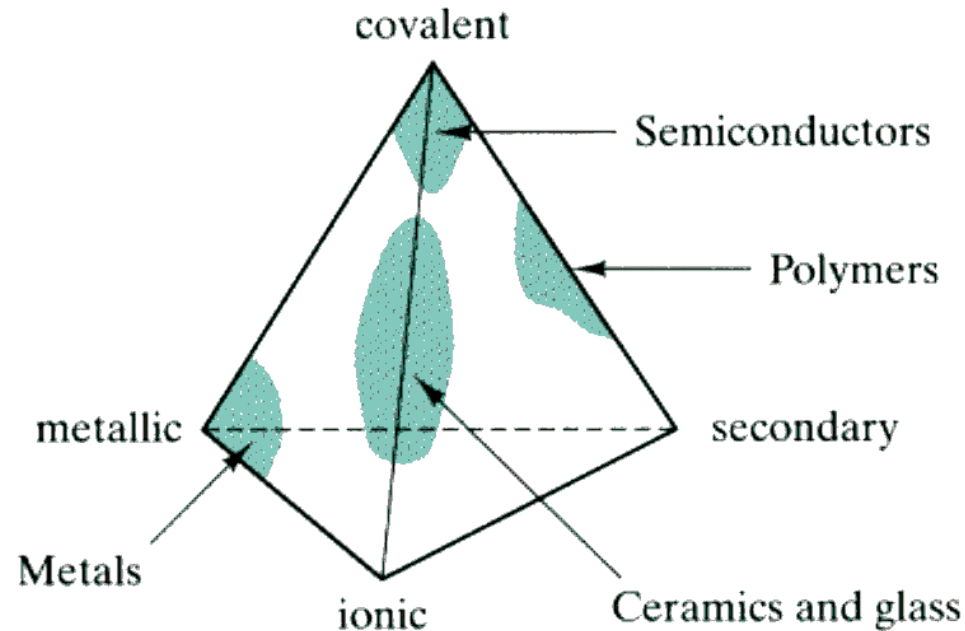
but α is smaller.

(thermal expansion coefficient)

Contents for previous class

Materials-Bonding Classification

Material type	Bonding character	Example
Metal	Metallic	Iron (Fe) and the ferrous alloys
Ceramics and glasses	Ionic/covalent	Silica (SiO ₂): crystalline and noncrystalline
Polymers	Covalent and secondary	Polyethylene $(-C_2H_4)_n$
Semiconductors	Covalent or covalent/ionic	Silicon (Si) or cadmium sulfide (CdS)



< 실제 많은 재료는 2개 혹은 그 이상의 결합에 혼합 >

Contents for previous class

Summary: Properties from Bonds

Ceramics

(Ionic & covalent bonding):

Large bond energy

large T_m

large E

small α

Metals

(Metallic bonding):

Variable bond energy

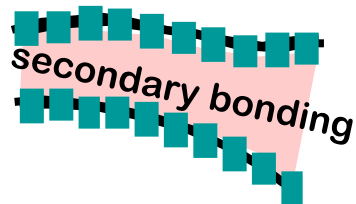
moderate T_m

moderate E

moderate α

Polymers

(Covalent & Secondary):



Directional Properties

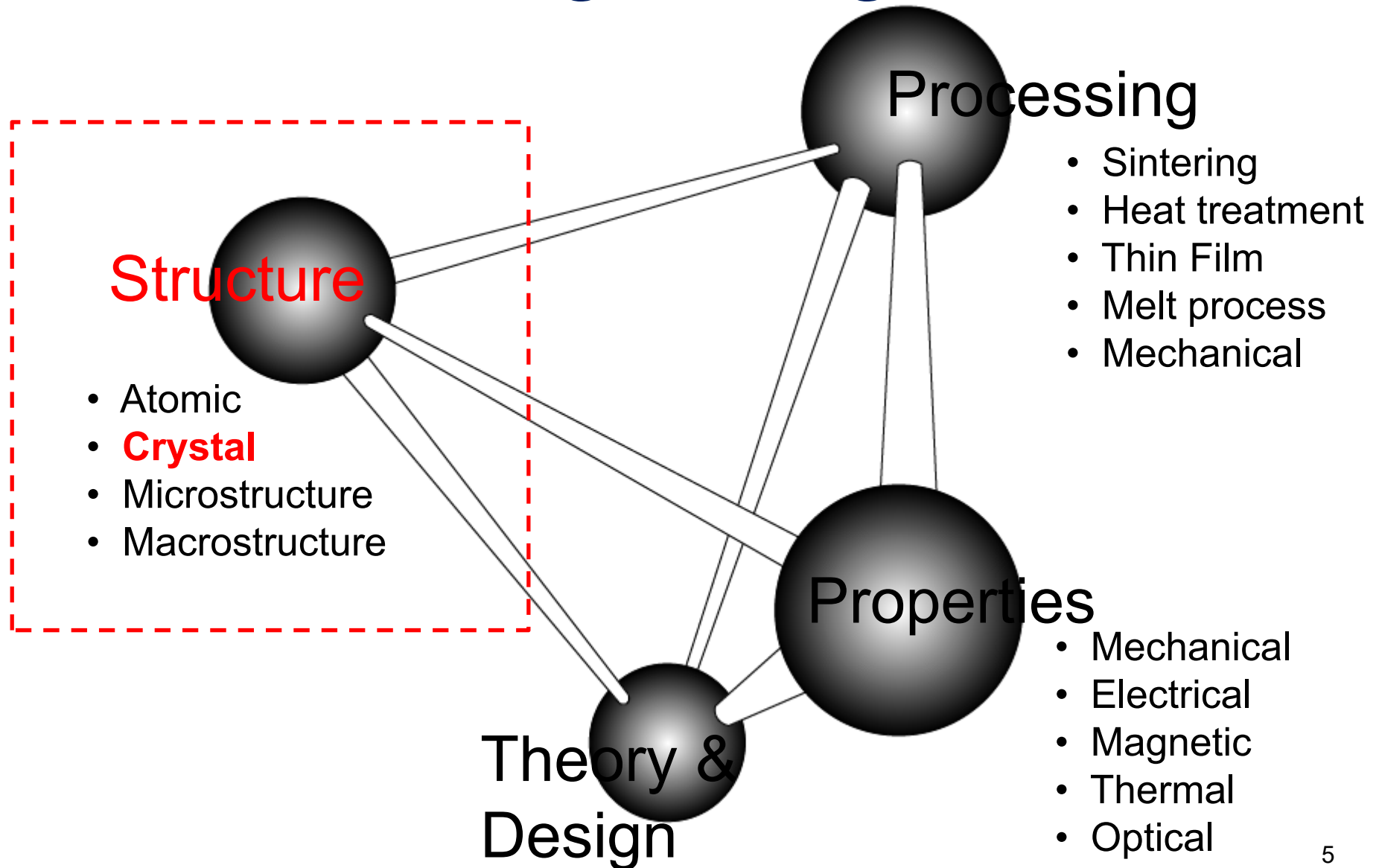
Secondary bonding dominates

small T_m

small E

large α

Materials Science and Engineering



Contents for today's class

CHAPTER 3:

Fundamentals of Crystallography

I. Crystal Structures

- Lattice, Unit Cells, Crystal system

II. Crystallographic Points, Directions, and Planes

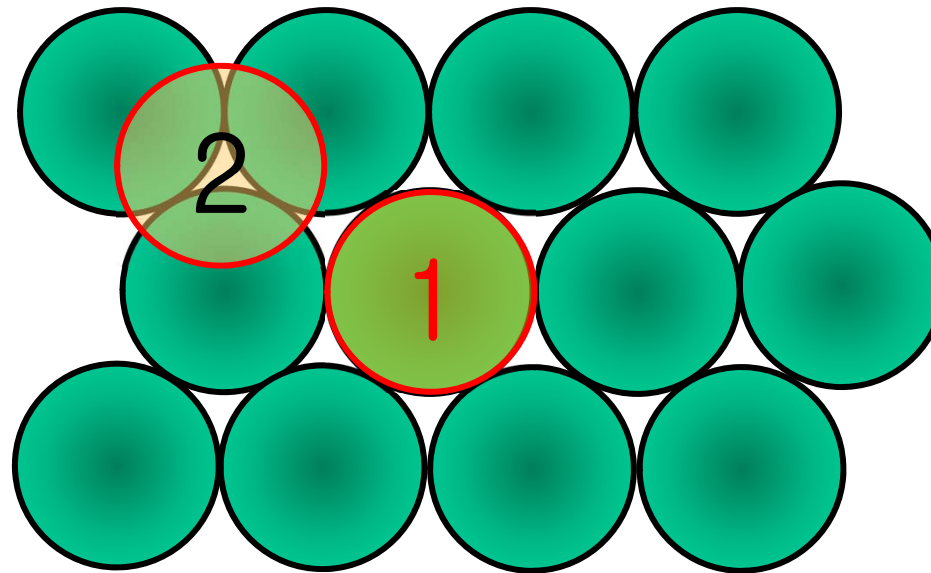
- Point coordinates, Crystallographic directions, Crystallographic planes

III. Crystalline and Noncrystalline Materials

- Single crystals, Polycrystalline materials, Anisotropy, Noncrystalline solids

Stacking of atoms in solid

Finding stable position

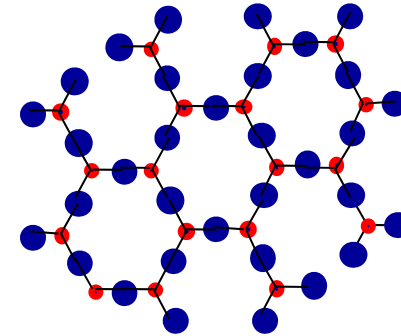


- Minimize energy configuration
 - Related to the bonding nature

Materials and Packing

Crystalline materials...

- atoms pack in periodic, 3D arrays
- typical of:
 - metals
 - many ceramics
 - some polymers



crystalline SiO₂

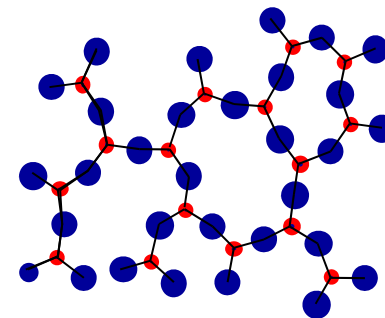
Adapted from Fig. 3.22(a),
Callister 7e.

Quasicrystalline materials...

Noncrystalline materials...

- atoms have no periodic packing
- occurs for:
 - complex structures
 - rapid cooling

• **Si** • **Oxygen**



noncrystalline SiO₂

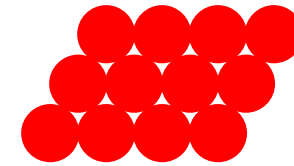
"Amorphous" = Noncrystalline

atomic arrangement in the solid state

➤ Solid materials are classified according to the **regularity** with which atoms and ions are arranged with respect to one another.

➤ So, how are they arranged ?

(a) **periodically** – having long range order in 3-D

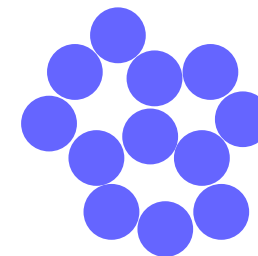


Crystal

(b) **quasi-periodically**

Quasicrystal

(c) **randomly** – having short range order with the characteristics of bonding type but losing the long range order



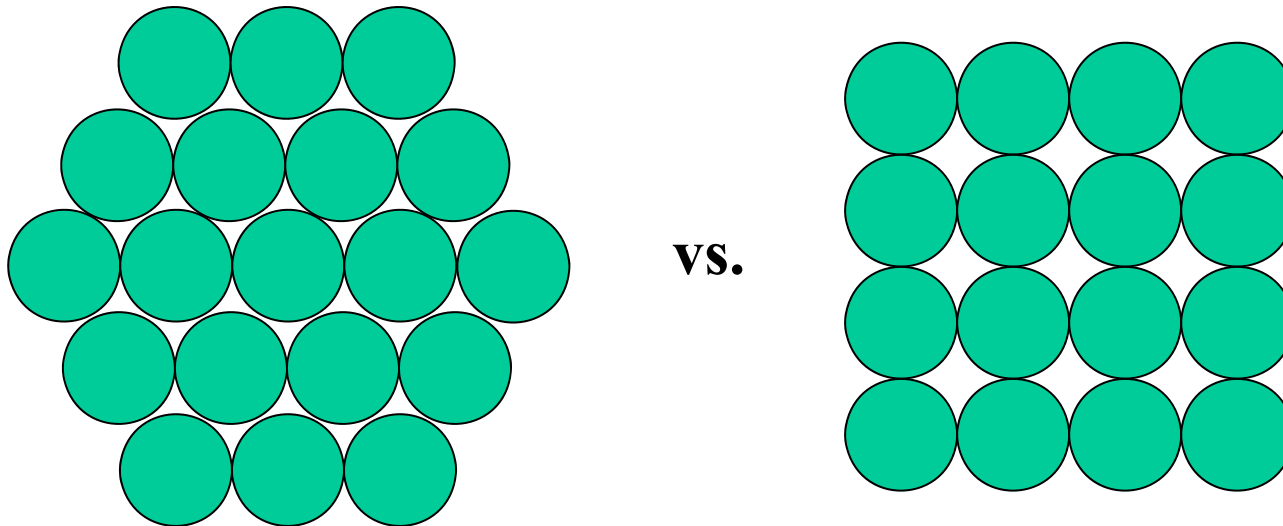
Amorphous

➤ **Crystal: Perfection → Imperfection**

I. Crystal structures

- How can we stack metal atoms to minimize empty space?

2-dimensions



Now stack these 2-D layers to make 3-D structures

Crystalline materials - three-dimensional periodic arrangement of atoms, ions, or molecules- **translational periodicity**

Crystal – related topics

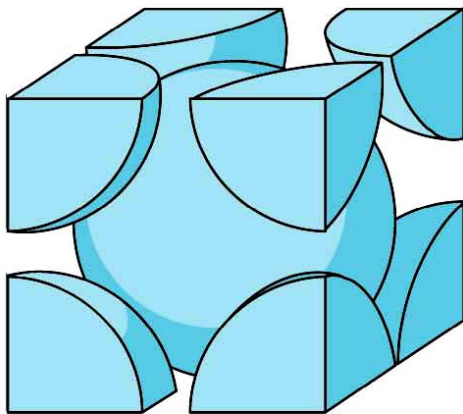
- Periodicity (주기성)
- Symmetry (대칭성)
- Anisotropy (비등방성)
- Directions and Planes (방향과 면)
- Interplanar spacing & angles (면간거리와 각도)
- Diffraction (회절)

I. Crystal structure

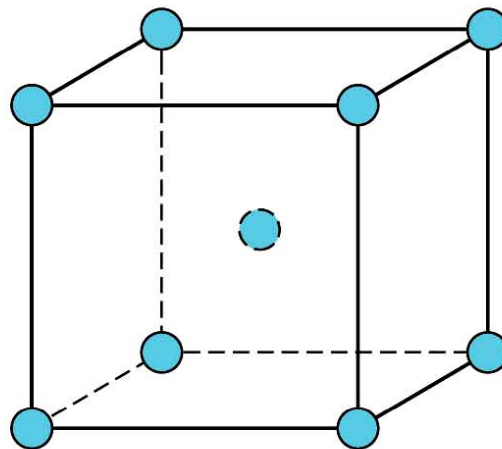
(1) Lattice : 결정 공간상에서 점들의 규칙적인 기하학적 배열

- 3D point array in space, such that each point has identical surroundings. These points may or may not coincide with atom positions.
- Simplest case : each atom \rightarrow its center of gravity \rightarrow point or space lattice \rightarrow pure mathematical concept

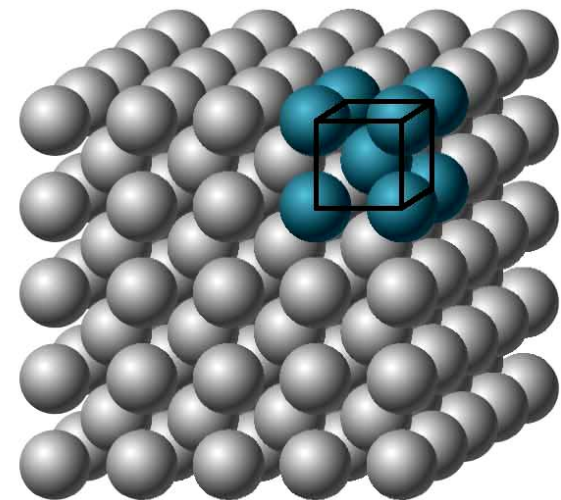
example: sodium (Na) ; body centered cubic



Hard-sphere unit cell



Reduced sphere unit cell

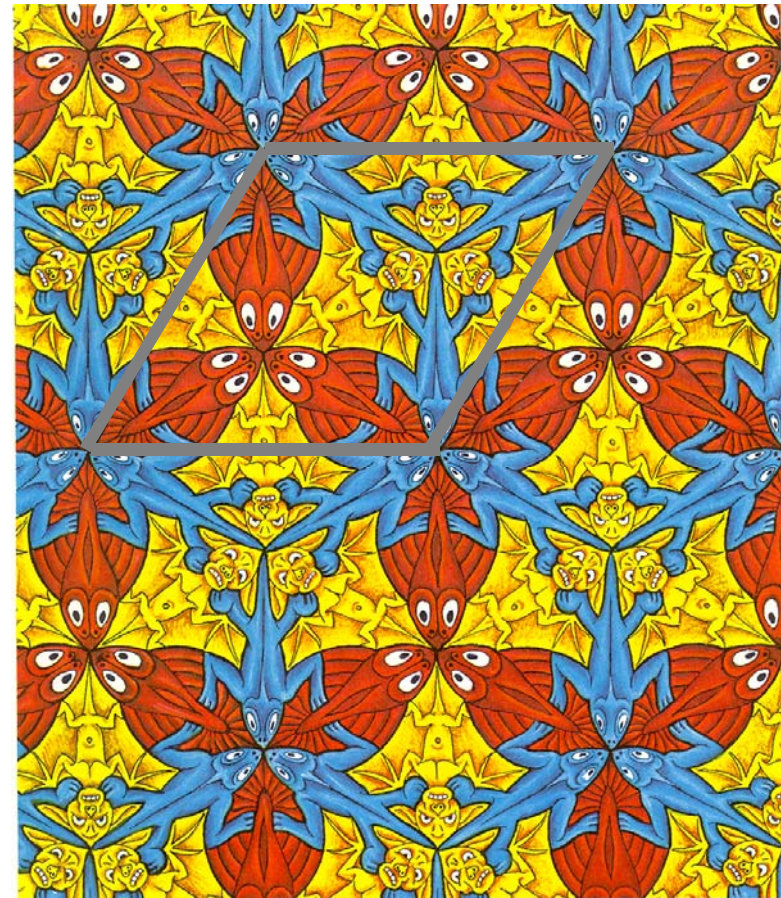
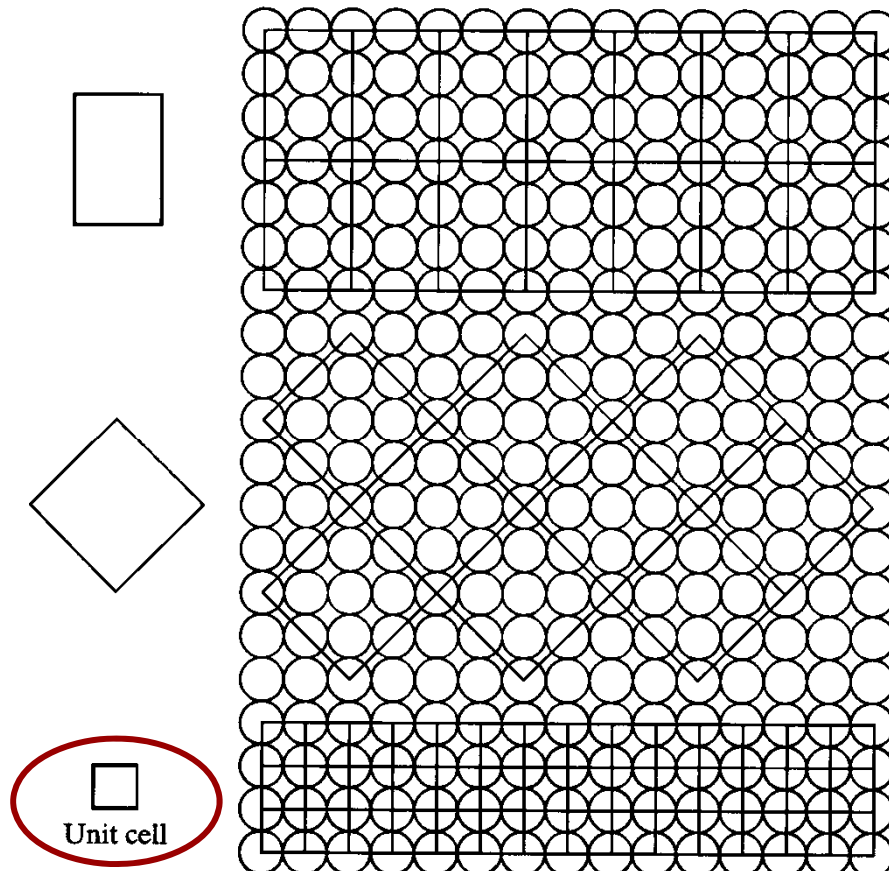


Aggregate of many atoms

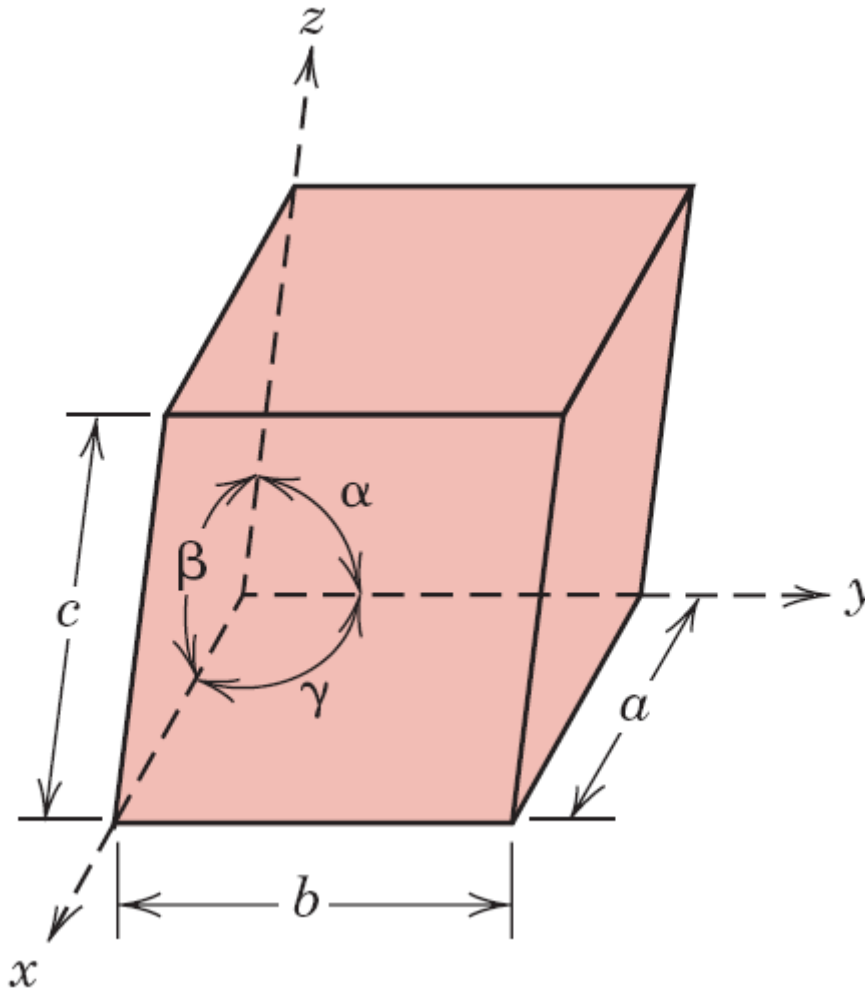
Chapter 3.3

(2) Unit cell

: smallest repetitive volume which contains the complete lattice pattern of a crystal



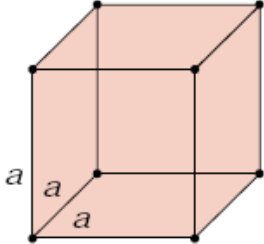
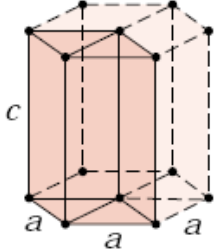
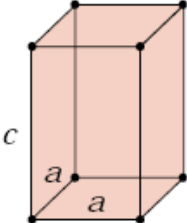
(3) Lattice parameter



length: a, b, c
angle: α, β, γ

(4) 7 crystal systems

Unit cell

<i>Crystal System</i>	<i>Axial Relationships</i>	<i>Interaxial Angles</i>	<i>Unit Cell Geometry</i>
Cubic	$a = b = c$	$\alpha = \beta = \gamma = 90^\circ$	
Hexagonal	$a = b \neq c$	$\alpha = \beta = 90^\circ, \gamma = 120^\circ$	
Tetragonal	$a = b \neq c$	$\alpha = \beta = \gamma = 90^\circ$	

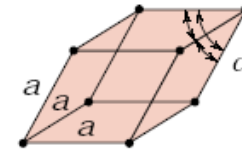
(4) 7 crystal systems (continued)

Unit cell

Rhombohedral

$$a = b = c$$

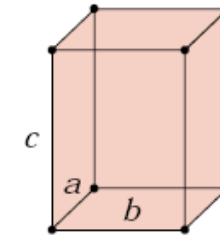
$$\alpha = \beta = \gamma \neq 90^\circ$$



Orthorhombic

$$a \neq b \neq c$$

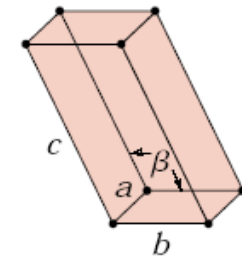
$$\alpha = \beta = \gamma = 90^\circ$$



Monoclinic

$$a \neq b \neq c$$

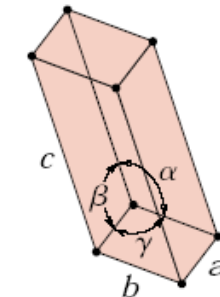
$$\alpha = \gamma = 90^\circ \neq \beta$$



Triclinic

$$a \neq b \neq c$$

$$\alpha \neq \beta \neq \gamma \neq 90^\circ$$



Unit cell

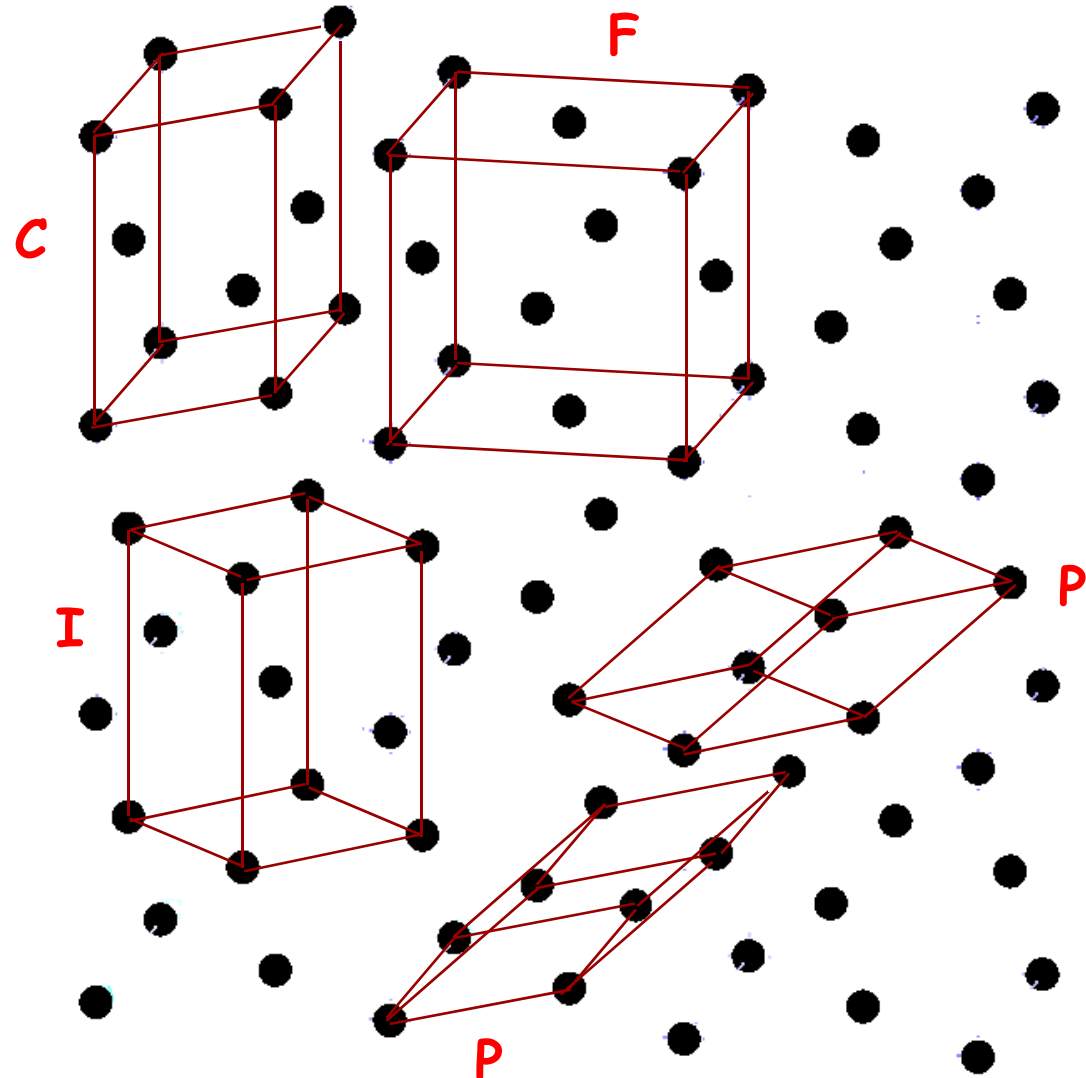
- **P, I, F, C**

- P : Primitive**

- I : Body centered**

- F : Face centered**

- C : Base centered**



Unit cell

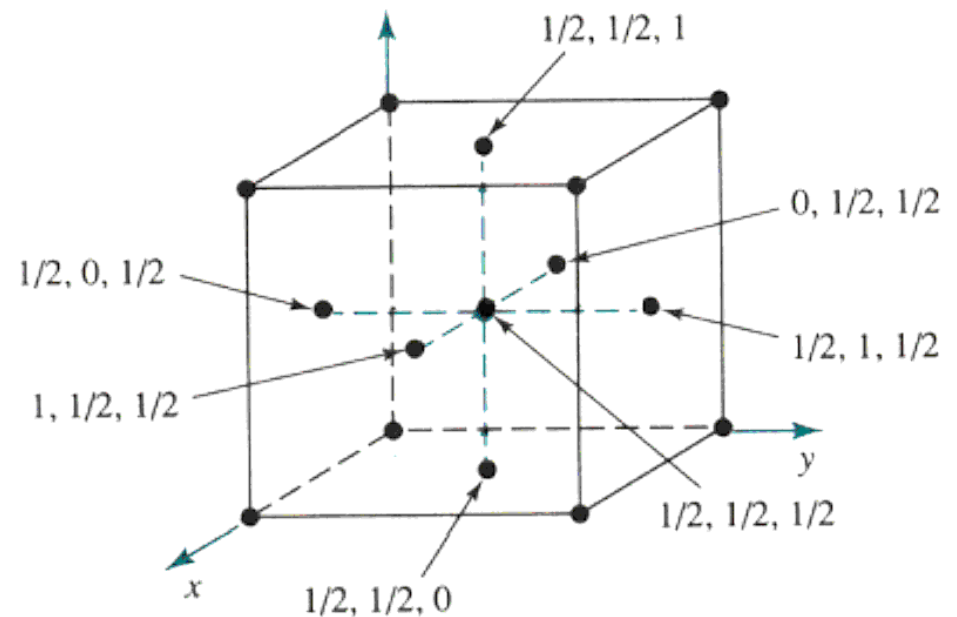
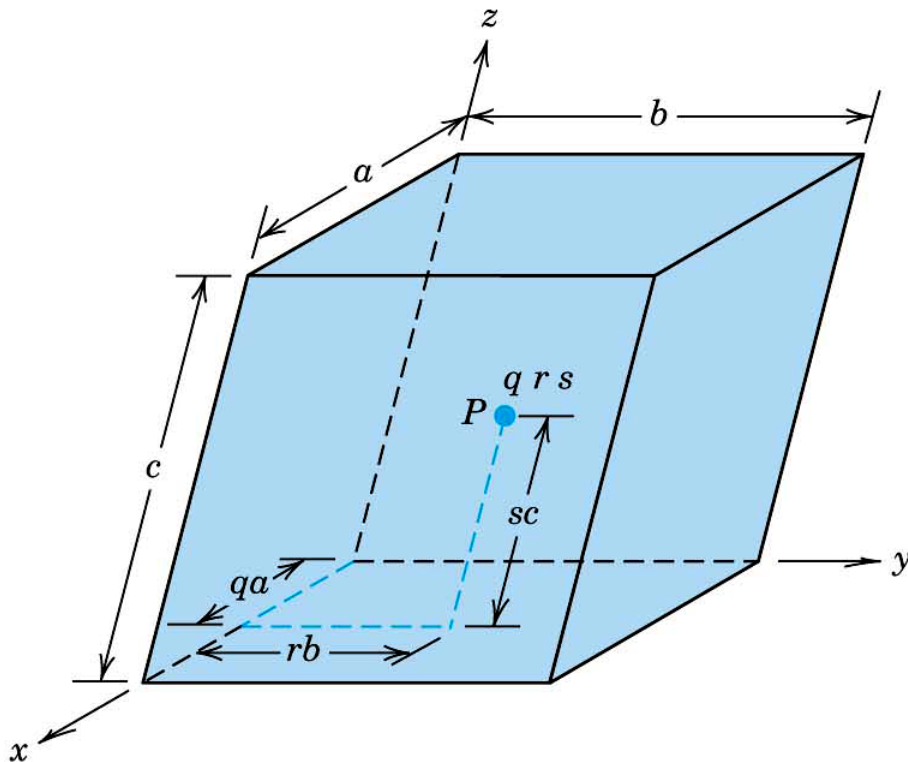
(5) 14 Bravais Lattice - Only 14 different types of unit cells are required to describe all lattices using symmetry

	cubic	hexagonal	rhombohedral (trigonal)	tetragonal	orthorhombic	monoclinic	triclinic
P							
I							
F							
C							

II. Crystallographic points, directions and planes

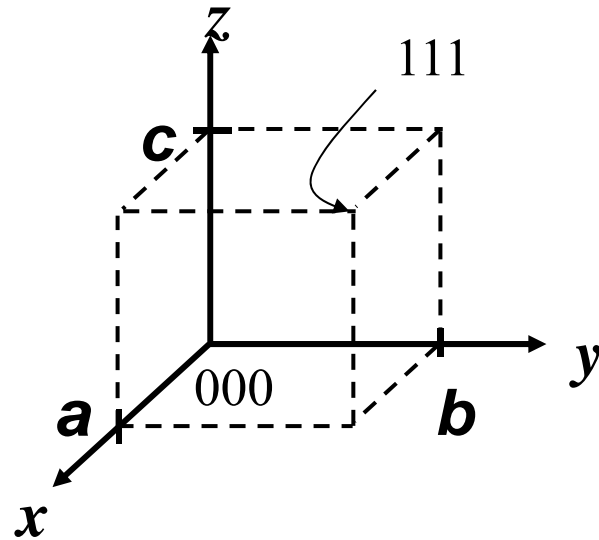
Chapter 3.5 Point coordinates

- position: fractional multiples of the unit cell edge lengths
 - ex) P: q, r, s



cubic unit cell

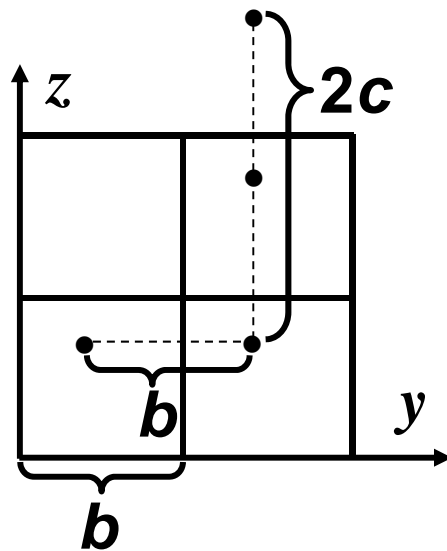
Chapter 3.5 Point coordinates



Point coordinates for unit cell center are

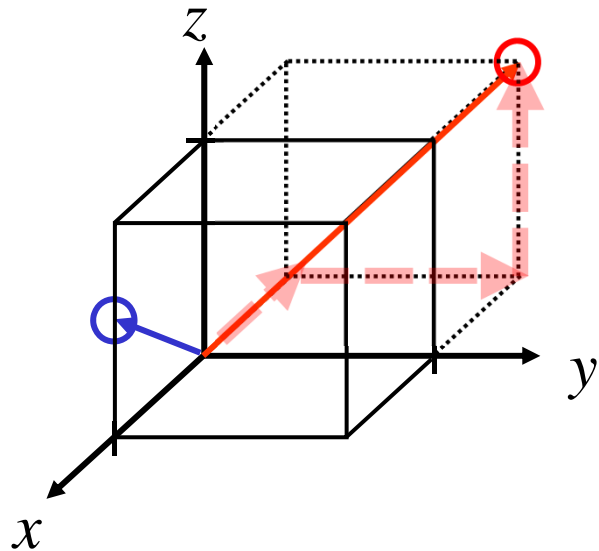
$$a/2, b/2, c/2 \quad \frac{1}{2}\frac{1}{2}\frac{1}{2}$$

Point coordinates for unit cell corner are 111



Translation: integer multiple of lattice constants \rightarrow identical position in another unit cell

Crystallographic Directions



Algorithm

1. Vector repositioned (if necessary) to pass through origin.
2. Read off projections in terms of unit cell dimensions a , b , and c
3. Adjust to smallest integer values
4. Enclose in square brackets, no commas

$$[uvw]$$

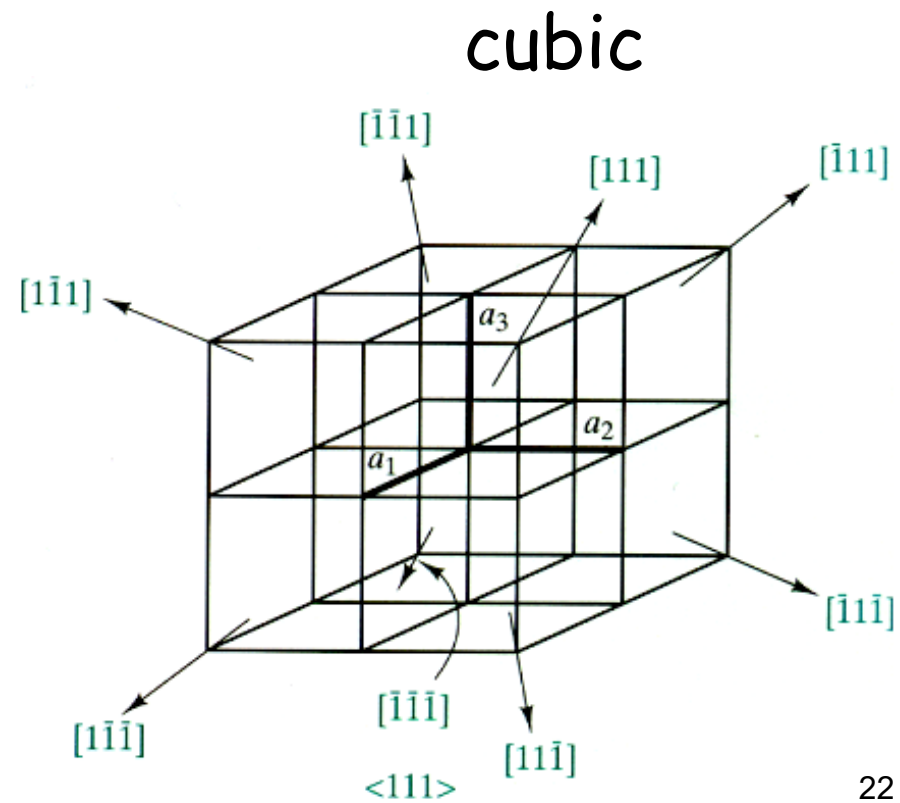
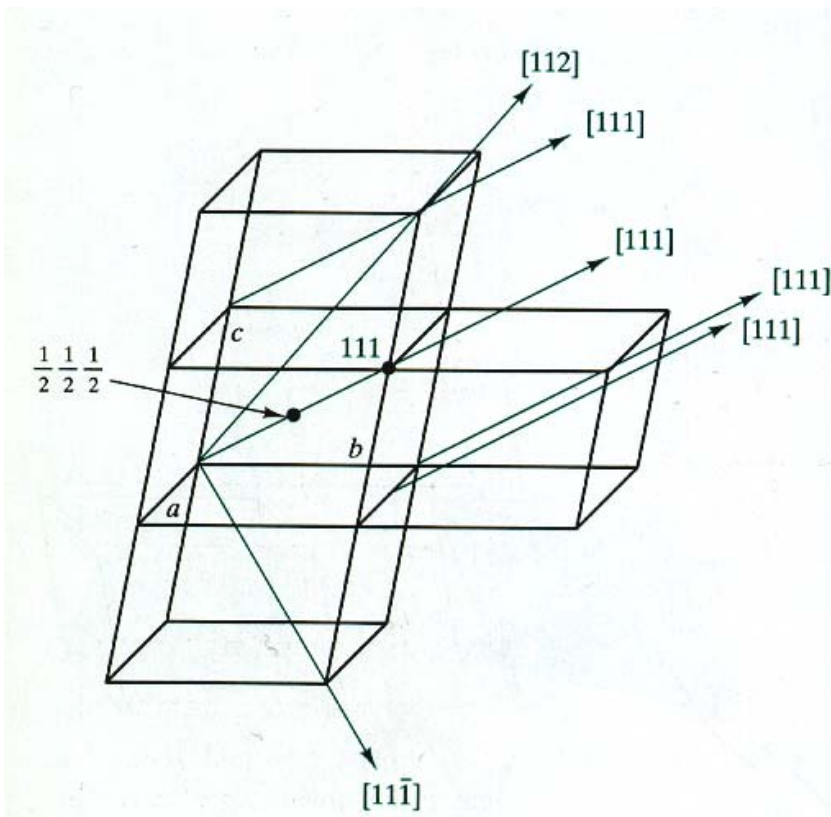
ex: $1, 0, \frac{1}{2} \Rightarrow 2, 0, 1 \Rightarrow [201]$

$-1, 1, 1 \Rightarrow [\bar{1}11]$ where overbar represents a negative index

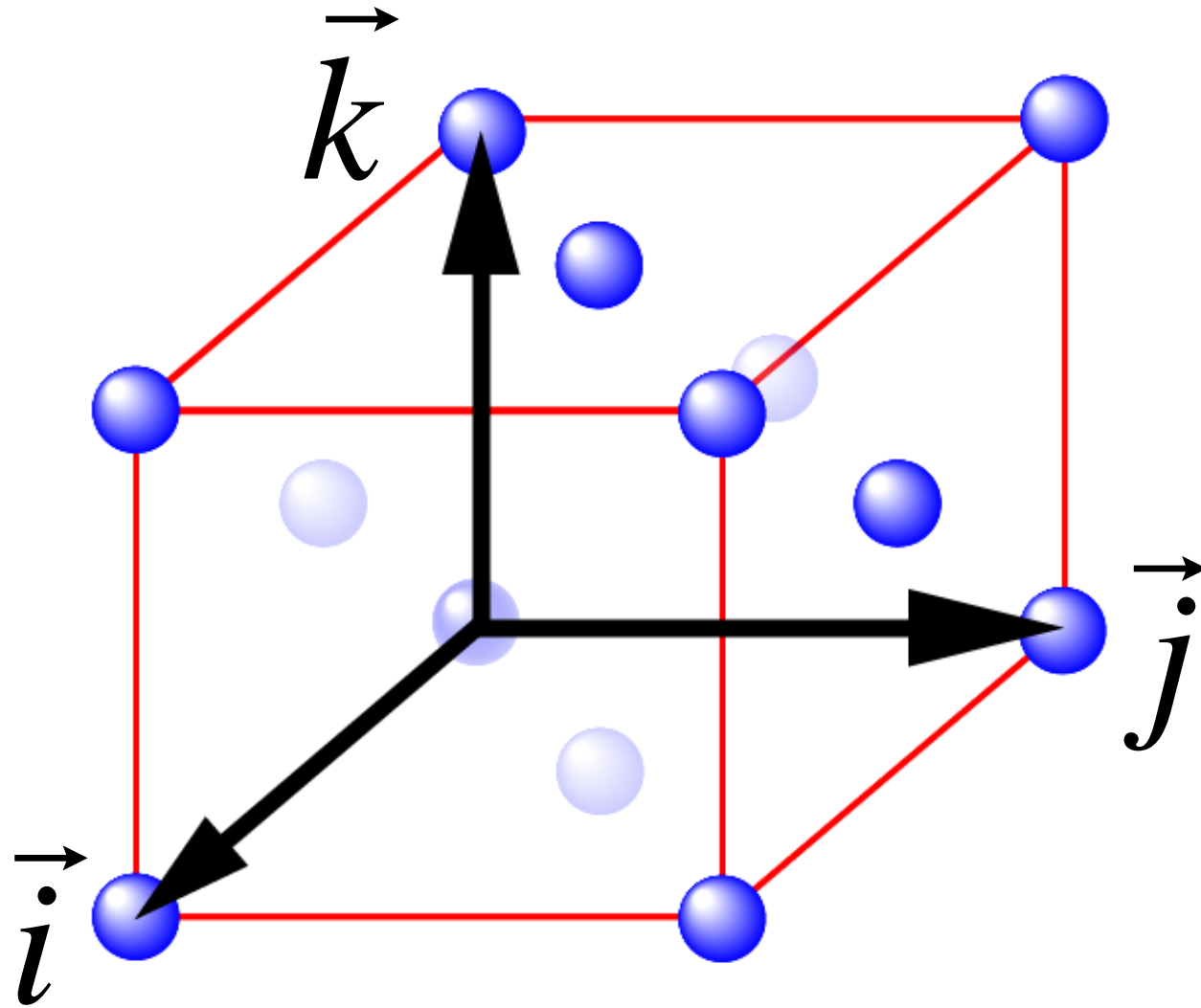
families of directions $\langle uvw \rangle$

Crystallographic Directions

- a line between two points or a vector
- $[uvw]$ square bracket, smallest integer
- families of directions: $\langle uvw \rangle$ angle bracket



Impose index coordination



Directional indices

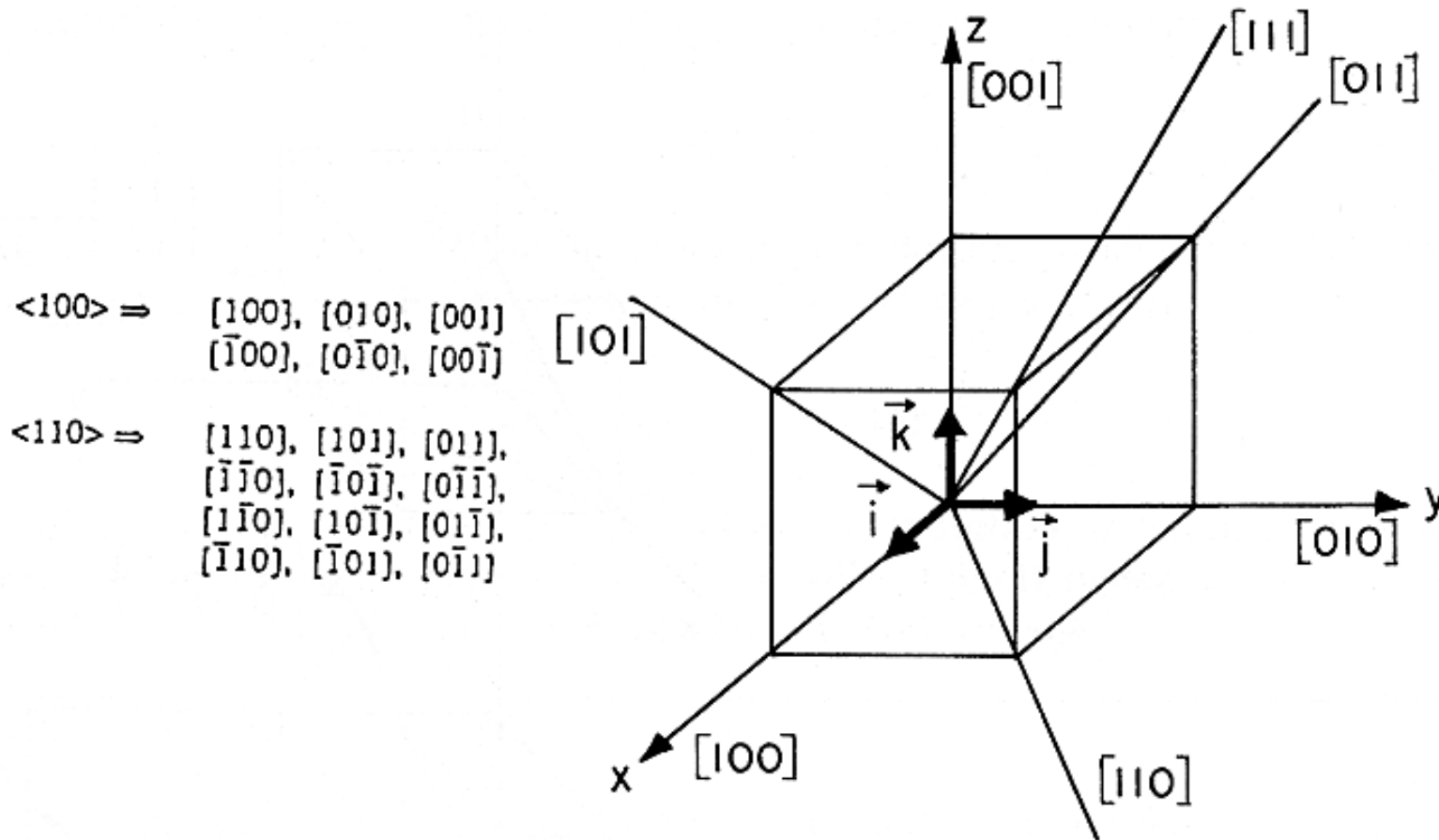
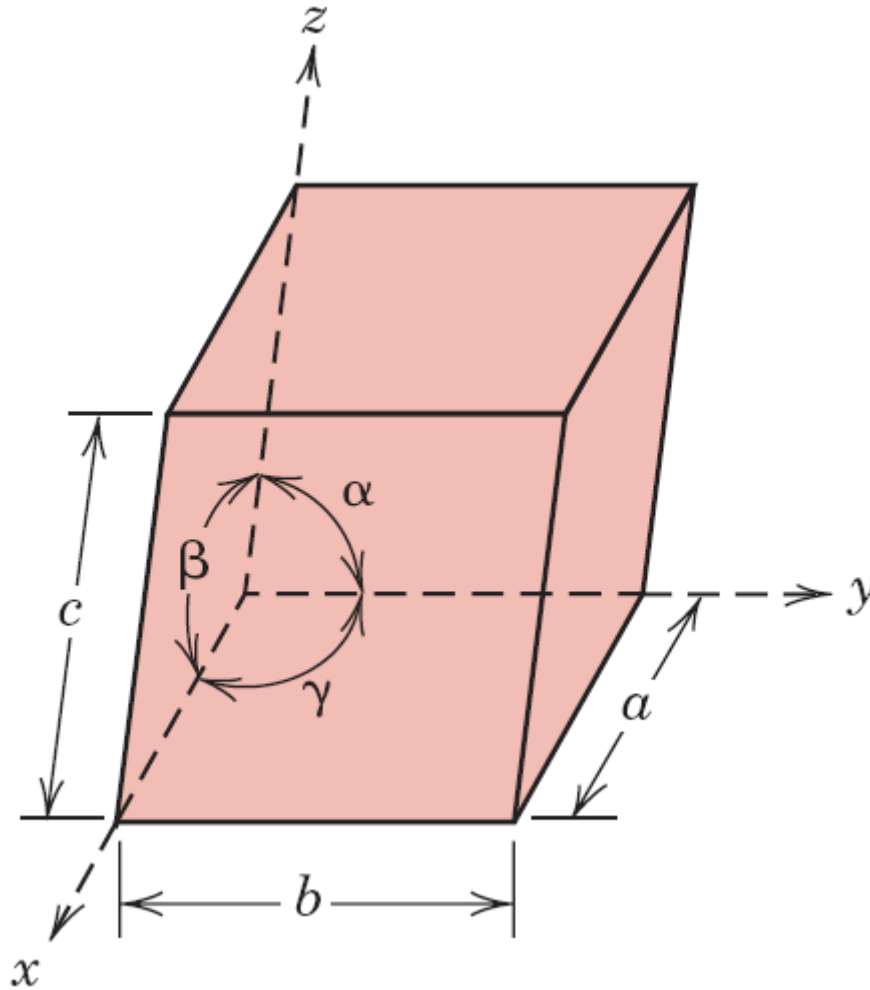


Figure 1.8 Directions in a cubic unit cell.

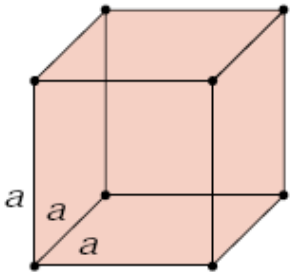
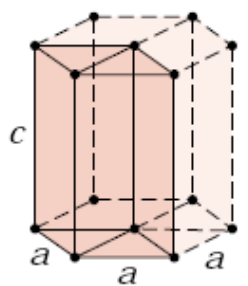
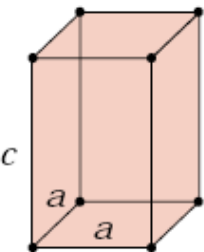
$\langle i j k \rangle$: permutation of $[i j k]$

Lattice Parameter



length: a, b, c
angle: α, β, γ

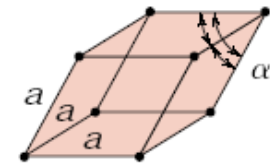
Table 3.6 Lattice Parameter Relationships and Figures Showing Unit Cell Geometries for the Seven Crystal Systems

<i>Crystal System</i>	<i>Axial Relationships</i>	<i>Interaxial Angles</i>	<i>Unit Cell Geometry</i>
Cubic	$a = b = c$	$\alpha = \beta = \gamma = 90^\circ$	
Hexagonal	$a = b \neq c$	$\alpha = \beta = 90^\circ, \gamma = 120^\circ$	
Tetragonal	$a = b \neq c$	$\alpha = \beta = \gamma = 90^\circ$	

Rhombohedral

$$a = b = c$$

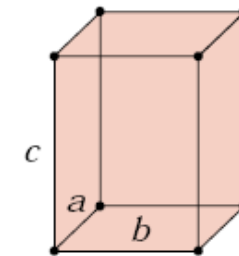
$$\alpha = \beta = \gamma \neq 90^\circ$$



Orthorhombic

$$a \neq b \neq c$$

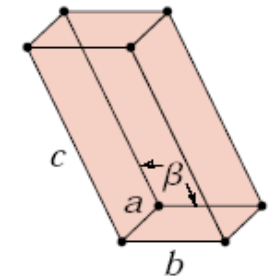
$$\alpha = \beta = \gamma = 90^\circ$$



Monoclinic

$$a \neq b \neq c$$

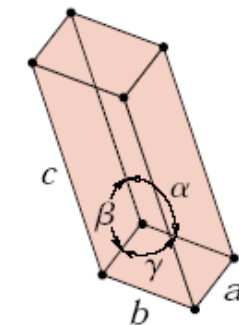
$$\alpha = \gamma = 90^\circ \neq \beta$$



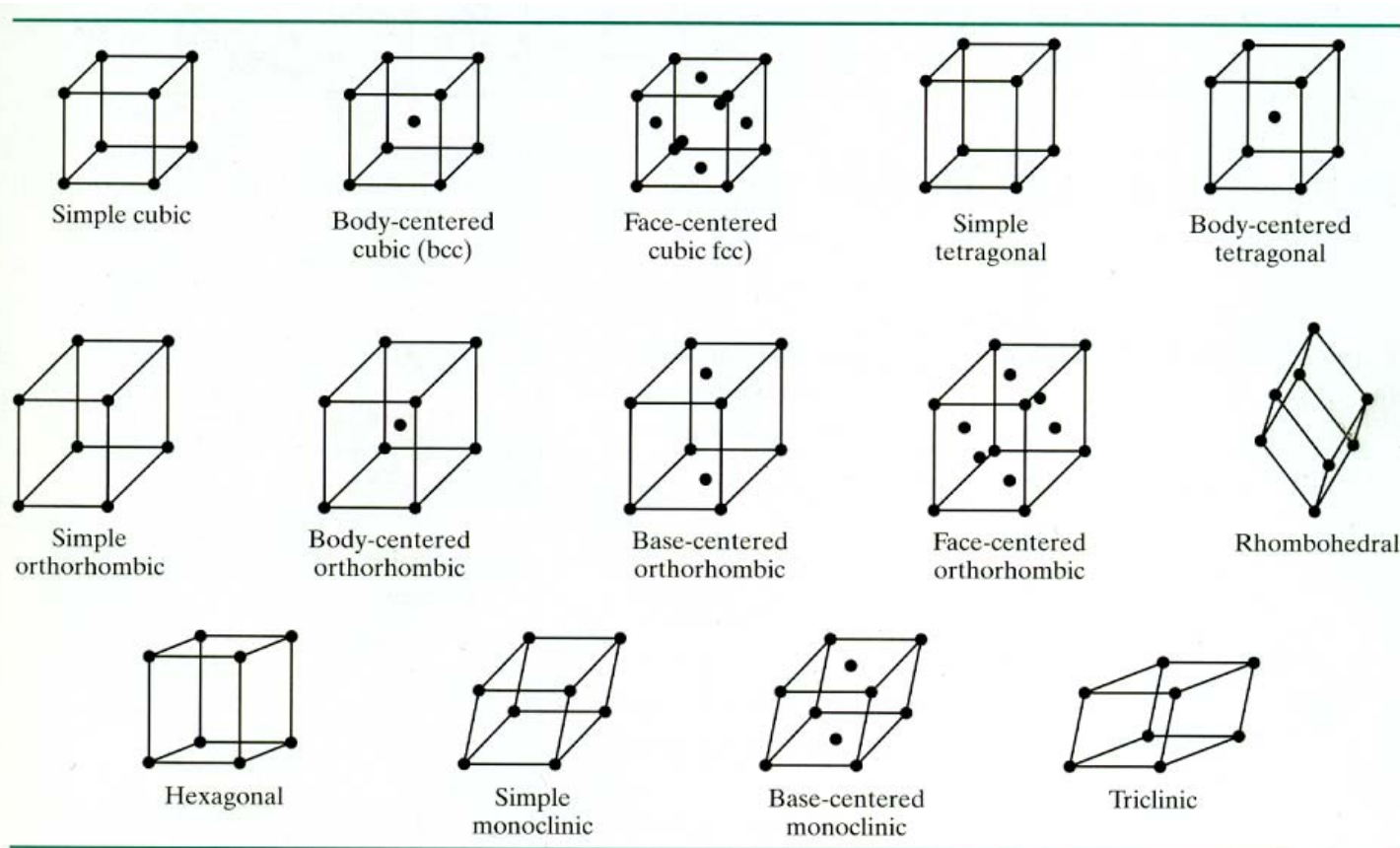
Triclinic

$$a \neq b \neq c$$

$$\alpha \neq \beta \neq \gamma \neq 90^\circ$$

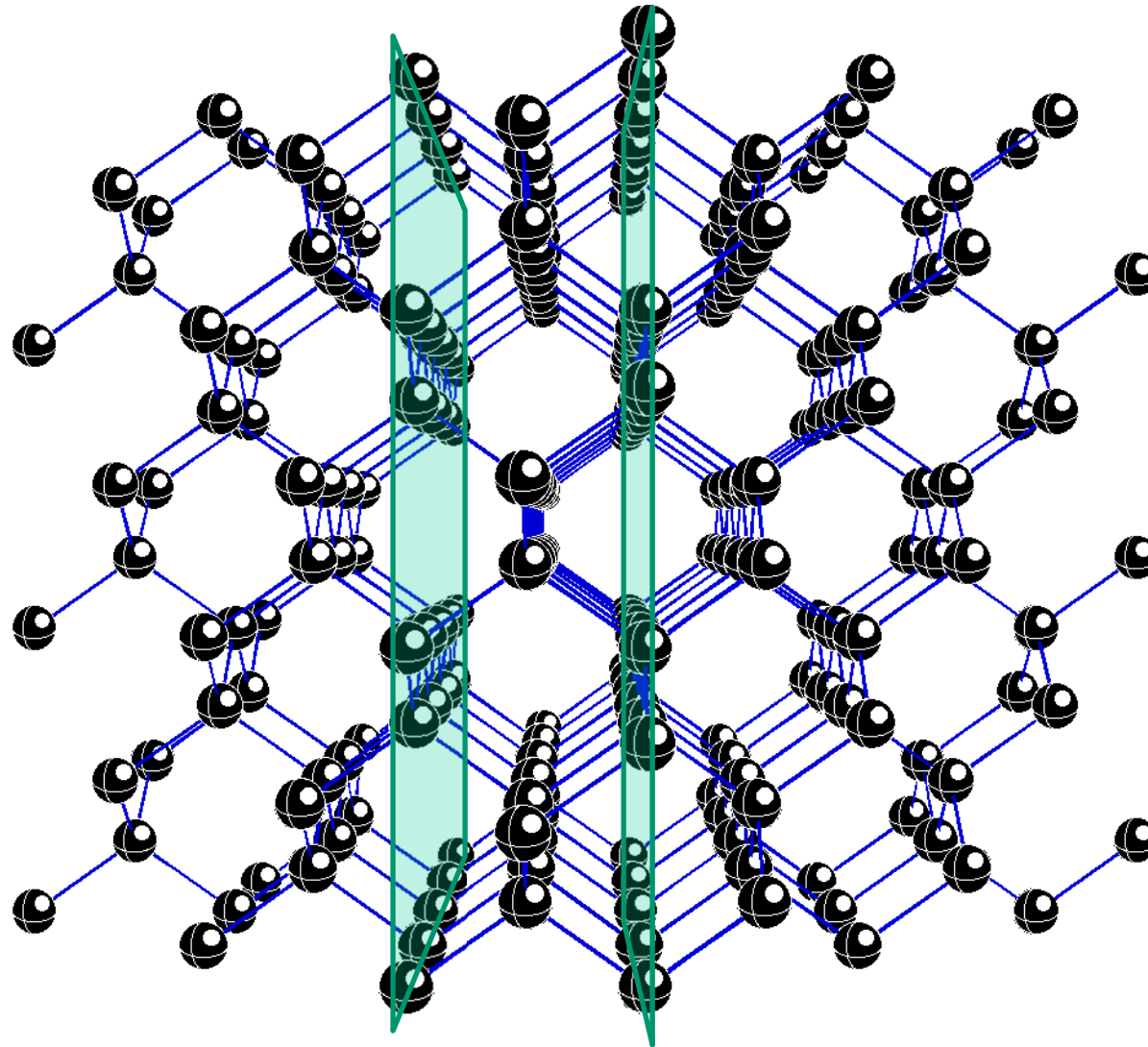


14 Bravais Lattice

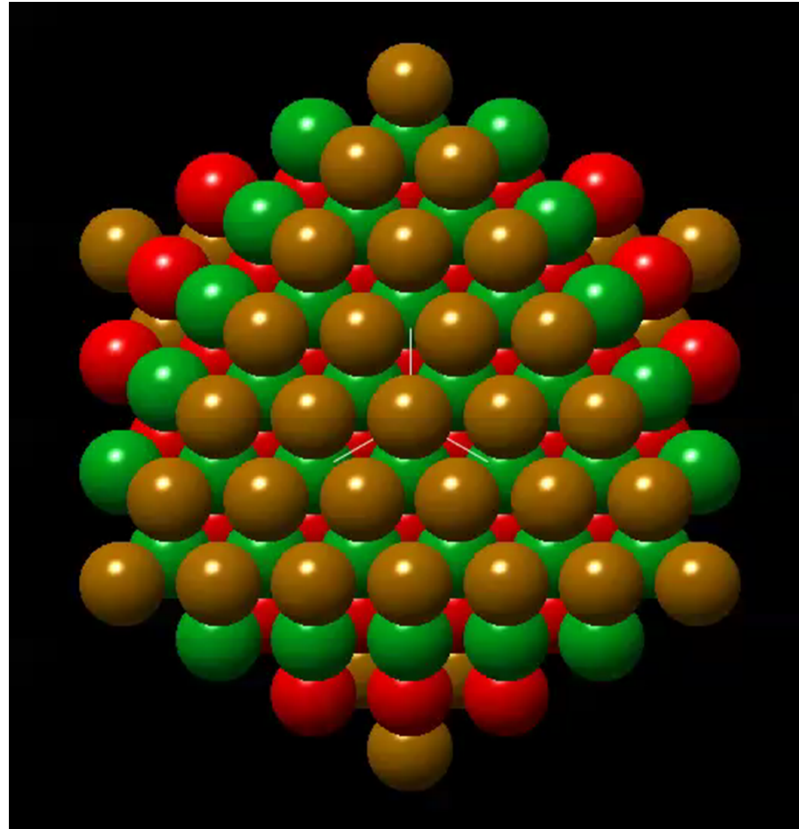


- Only 14 different types of unit cells are required to describe all lattices using symmetry
- simple (1), body-centered (2), base-centered (2) face-centered (4 atoms/unit cell)

Crystal view -Silicon

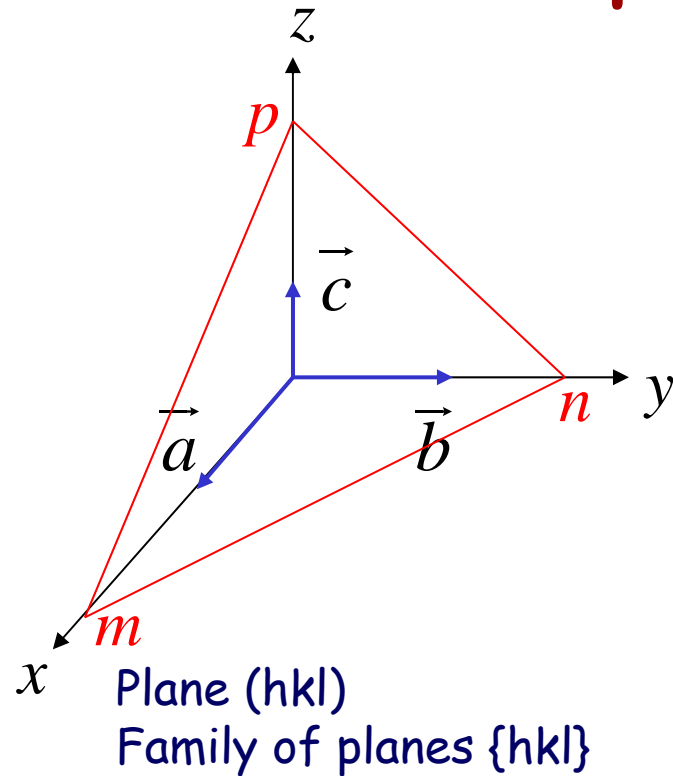


Crystallographic planes



Chapter 3.7 Crystallographic Planes

Lattice plane (Miller indices)

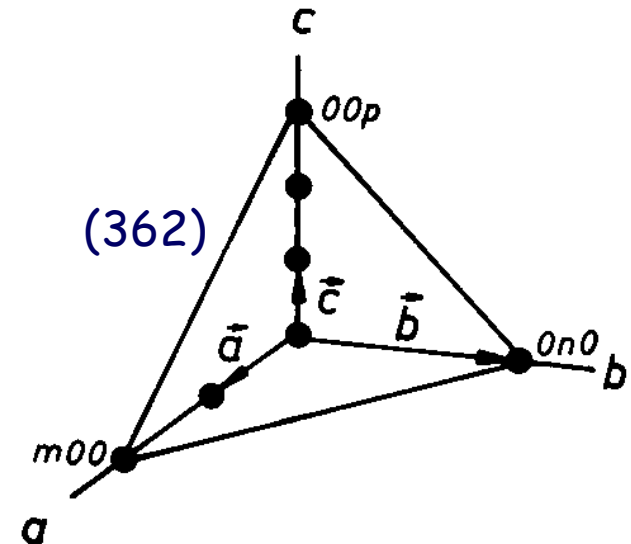


$m00, 0n0, 00p$: define lattice plane

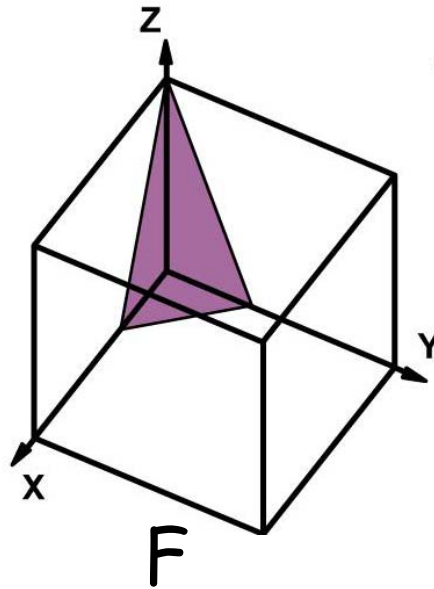
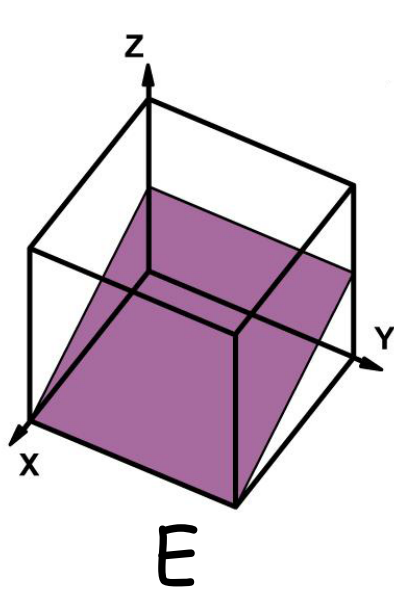
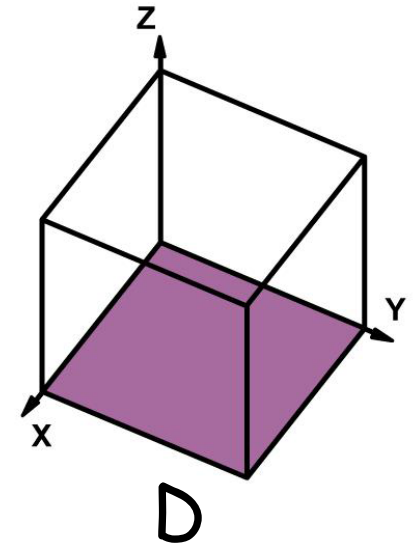
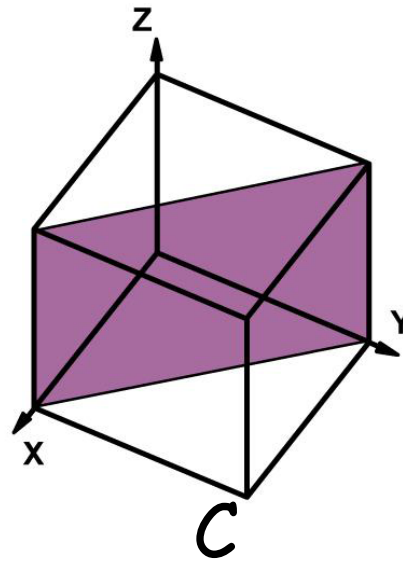
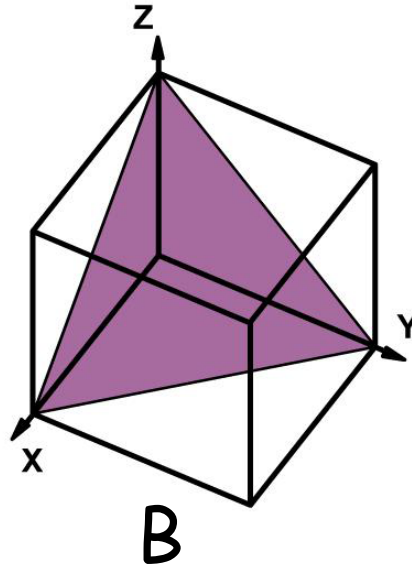
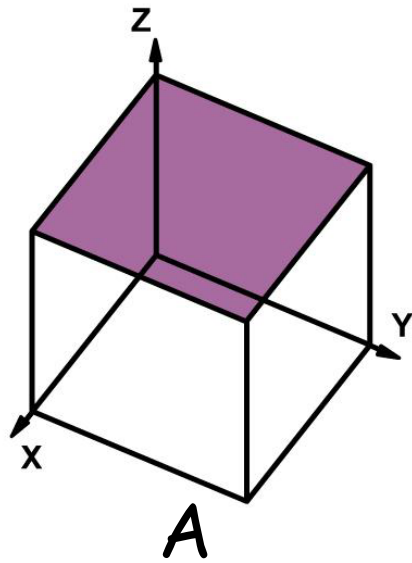
m, n, ∞ : no intercepts with axes

Intercepts @ (mnp)	2	1	3
Reciprocals	$\frac{1}{2}$	1	$\frac{1}{3}$
Miller indices	3	6	2
(362) plane			

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

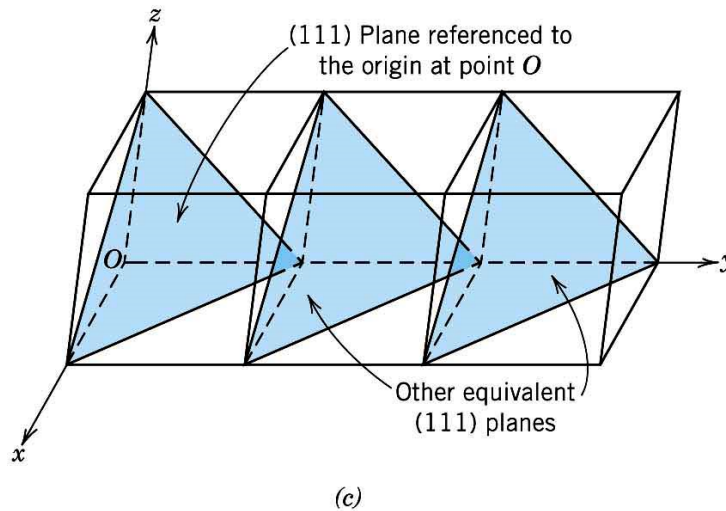
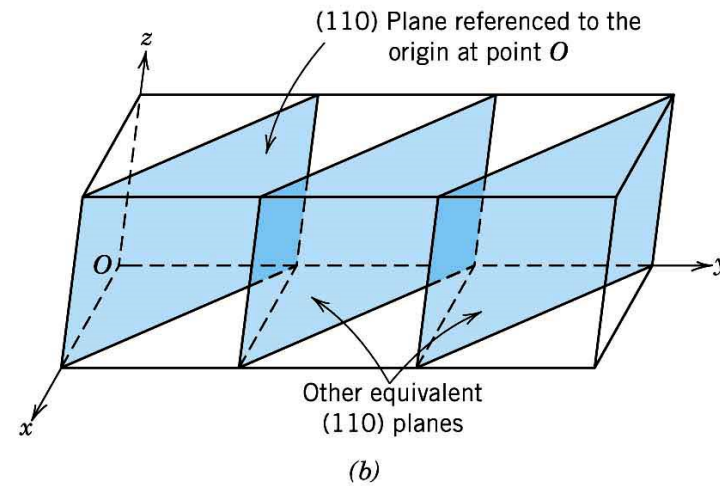
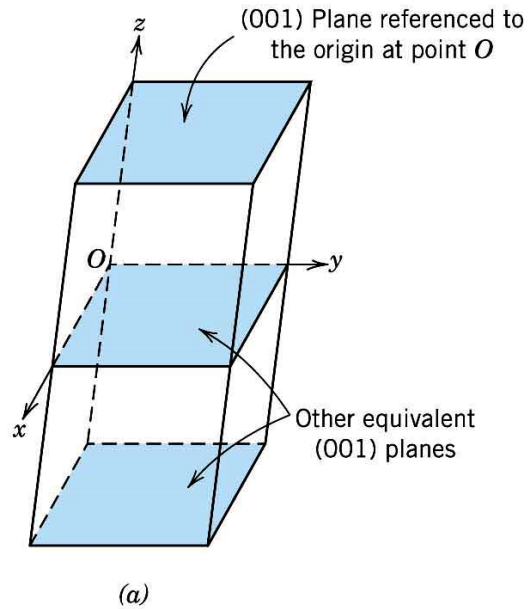


Crystallographic Planes

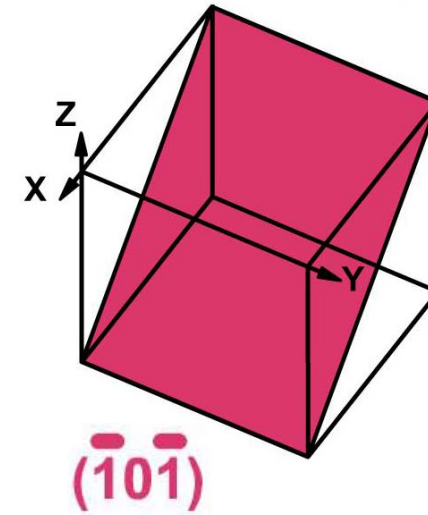
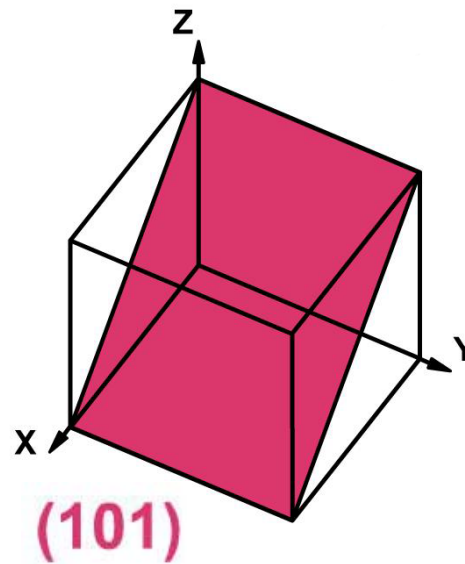
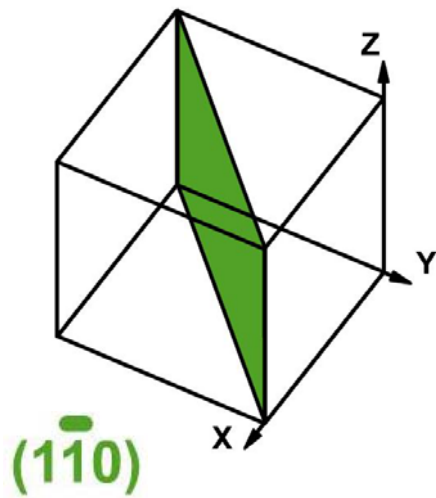
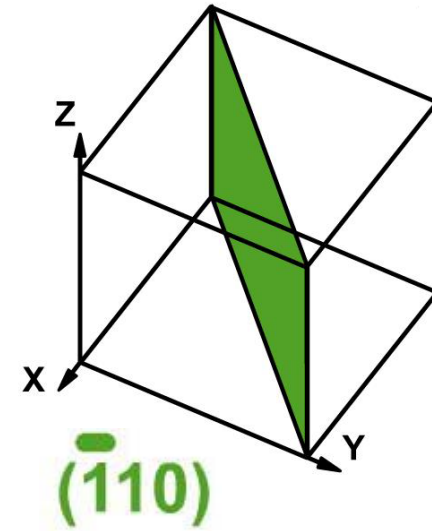
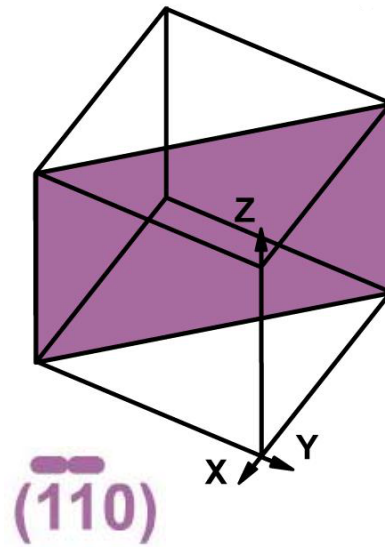
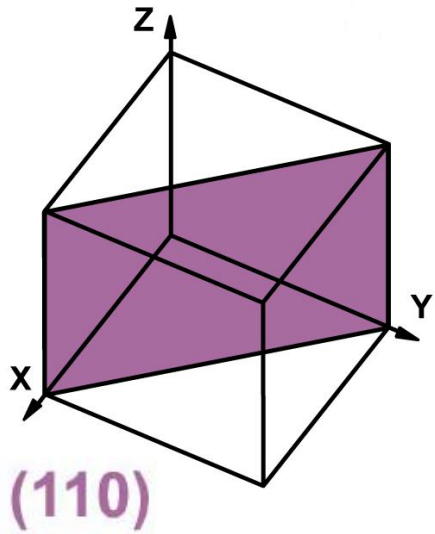


Plane	Intercepts	Indices
A	$\infty, \infty, 1$	(001)
B	1, 1, 1	(111)
C	1, 1, ∞	(110)
D	$\infty, \infty, -1$	(00 $\bar{1}$)
E	1, $\infty, 1/2$	()
F	1/3, 1/3, 1	()

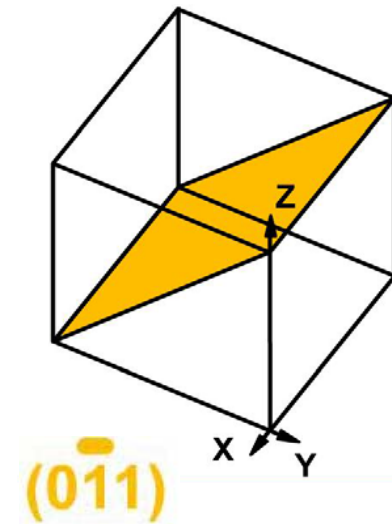
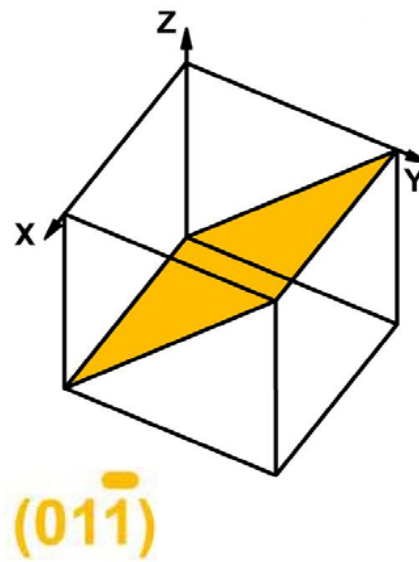
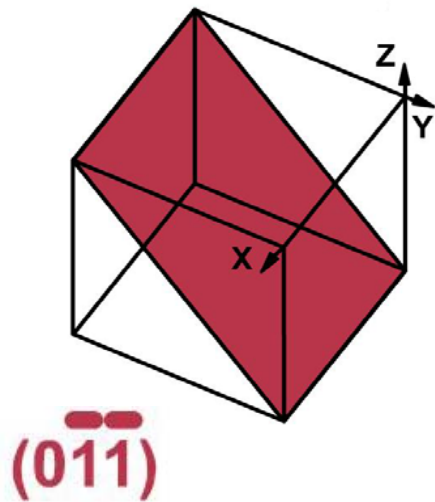
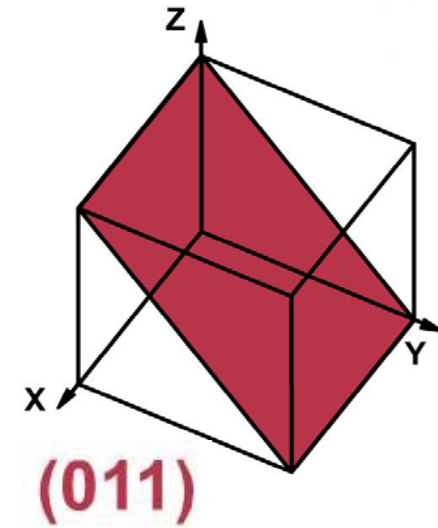
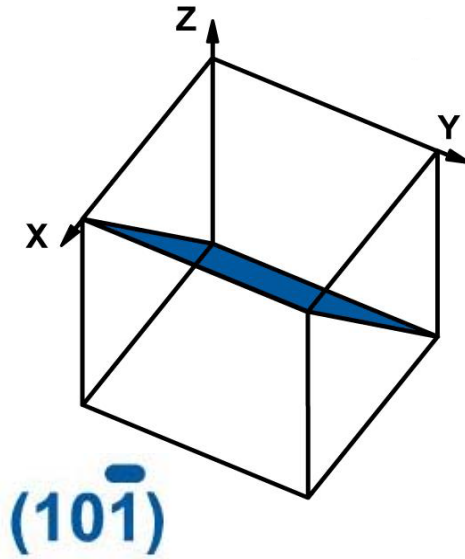
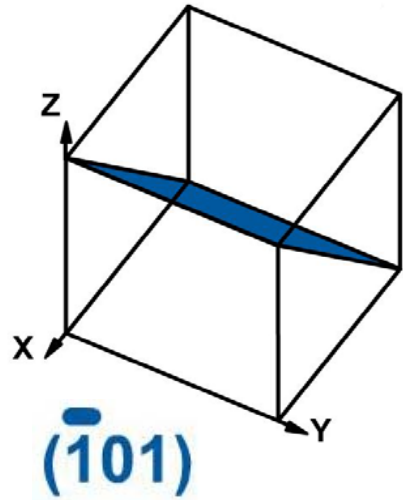
Crystallographic Planes



{110} Family



{110} Family



Directions, Planes, and Family

- **line, direction**
 - $[111]$ square bracket
 - $\langle 111 \rangle$ angular bracket - family

- **Plane**
 - (111) round bracket (Parentheses)
 - $\{111\}$ braces - family

HCP Crystallographic Directions

- Hexagonal Crystals

- 4 parameter Miller-Bravais lattice coordinates are related to the direction indices (i.e., $u'v'w'$) as follows.

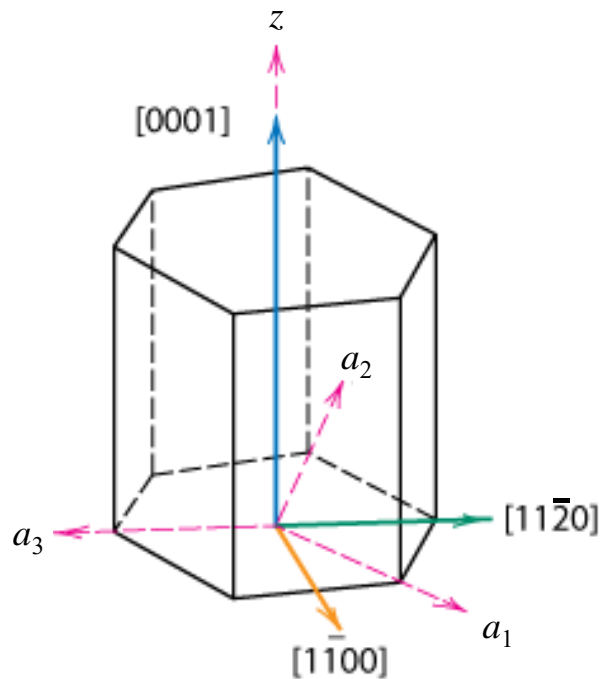


Fig. 3.8(a), Callister 7e.

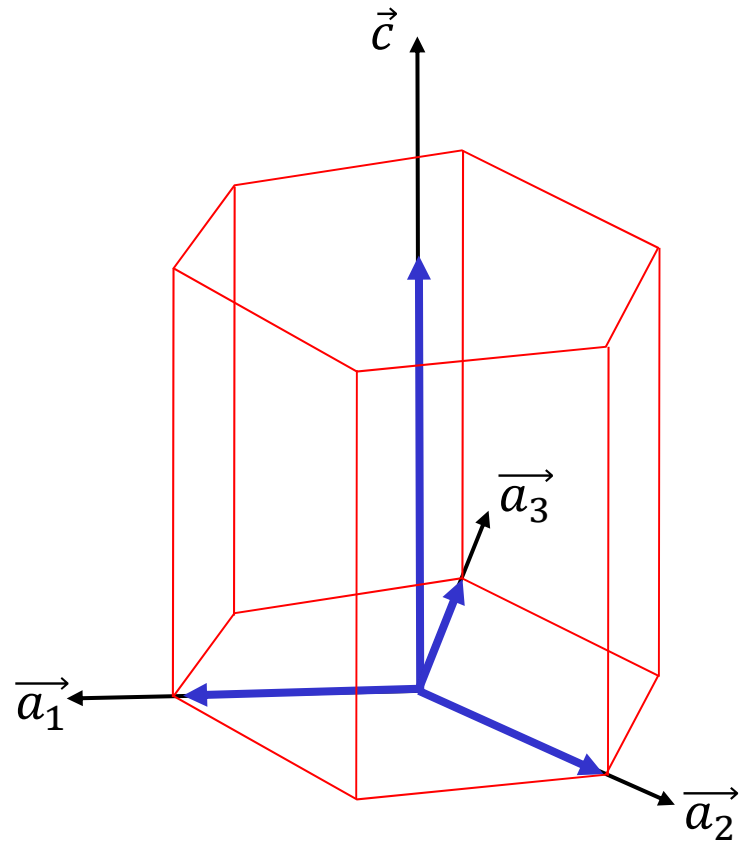
$$[u'v'w'] \rightarrow [uvw]$$

$$u = \frac{1}{3}(2u' - v')$$

$$v = \frac{1}{3}(2v' - u')$$

$$t = -(u + v)$$

$$w = w'$$



Miller index $[100]$

$$u = \frac{1}{3}(2u' - v')$$

$$v = \frac{1}{3}(2v' - u')$$

$$w = w'$$

$$u = \frac{2}{3}$$

$$v = \frac{-1}{3}$$

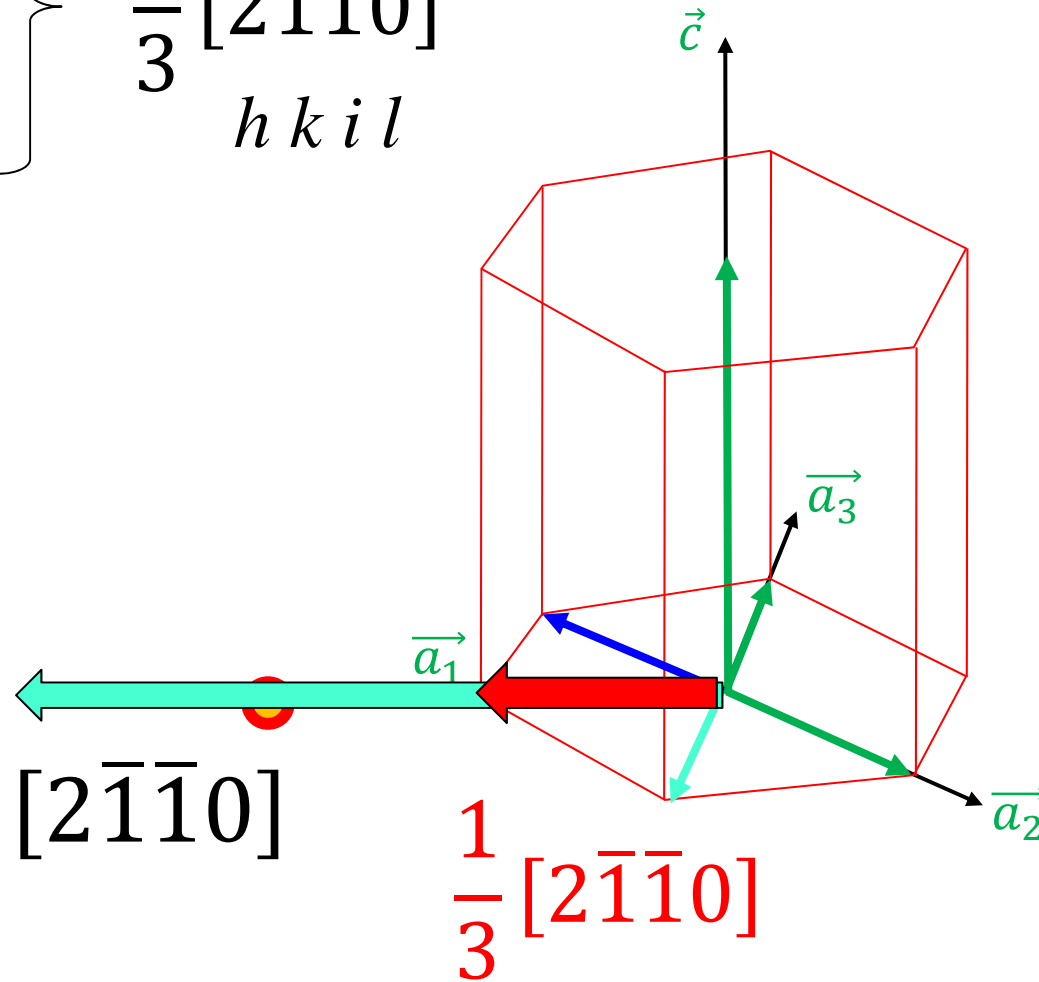
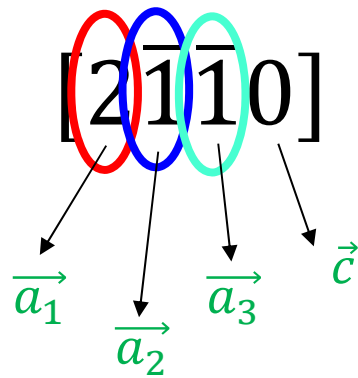
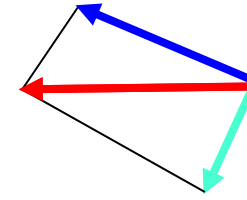
$$w = 0$$

Miller-Bravais index

$$\frac{1}{3} [2\bar{1}\bar{1}0]$$

$h k i l$

$i = -(h+k)$



Miller index $[101]$

$$u = \frac{1}{3}(2u' - v')$$

$$v = \frac{1}{3}(2v' - u')$$

$$w = w'$$

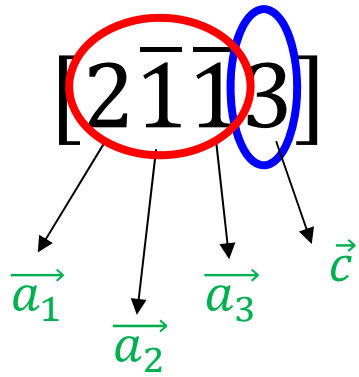
$$u = \frac{2}{3}$$

$$v = \frac{-1}{3}$$

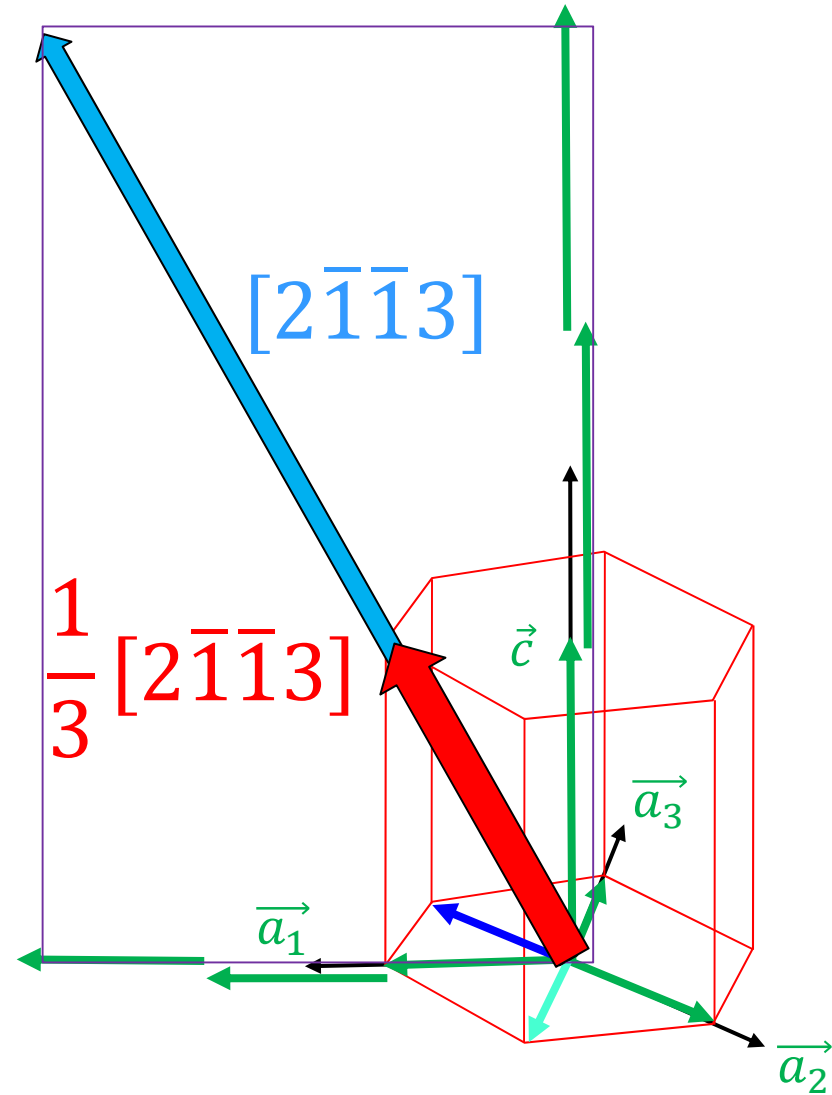
$$w = 1$$

Miller-Bravais index

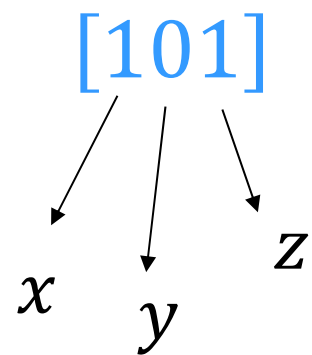
$$\frac{1}{3} [2\bar{1}\bar{1}3]$$



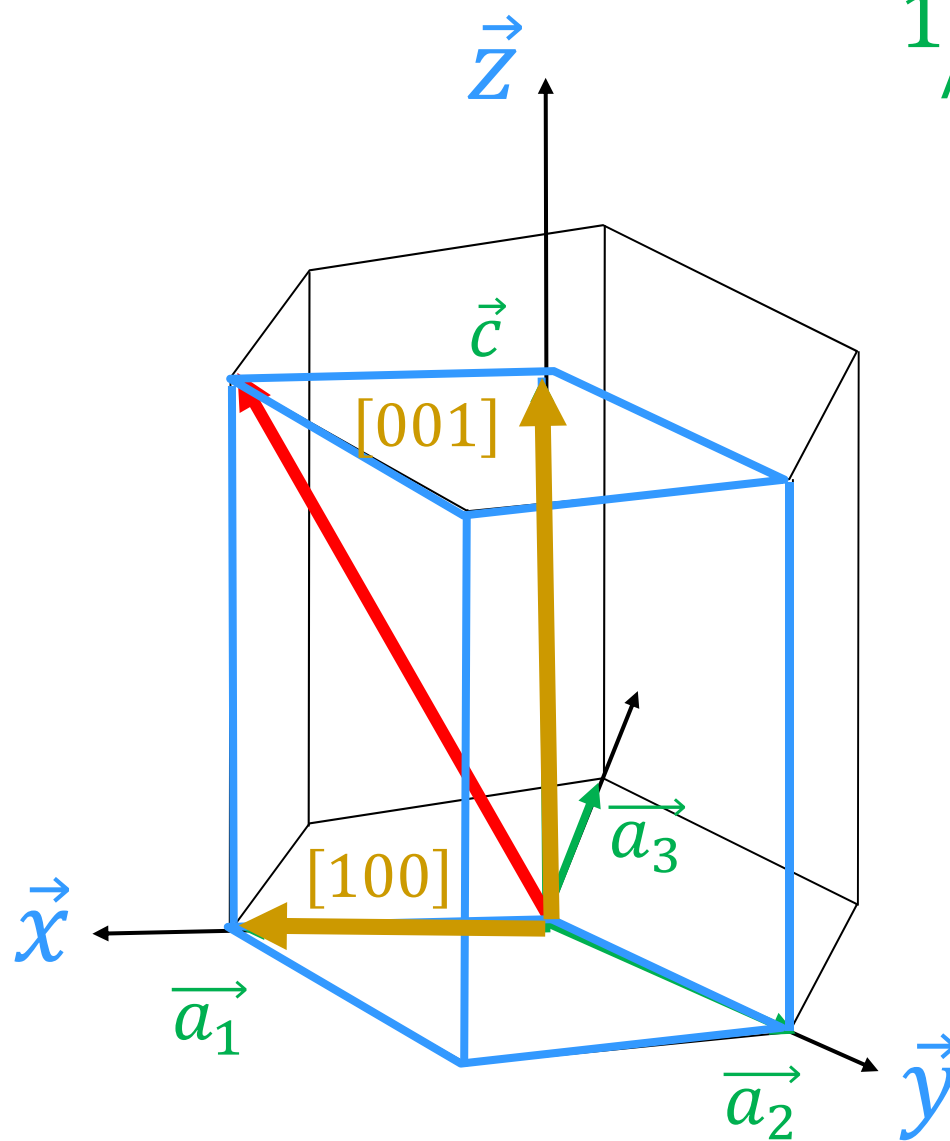
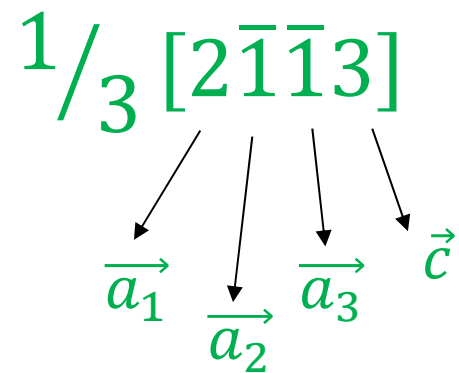
$[2\bar{1}\bar{1}0]$



Miller index

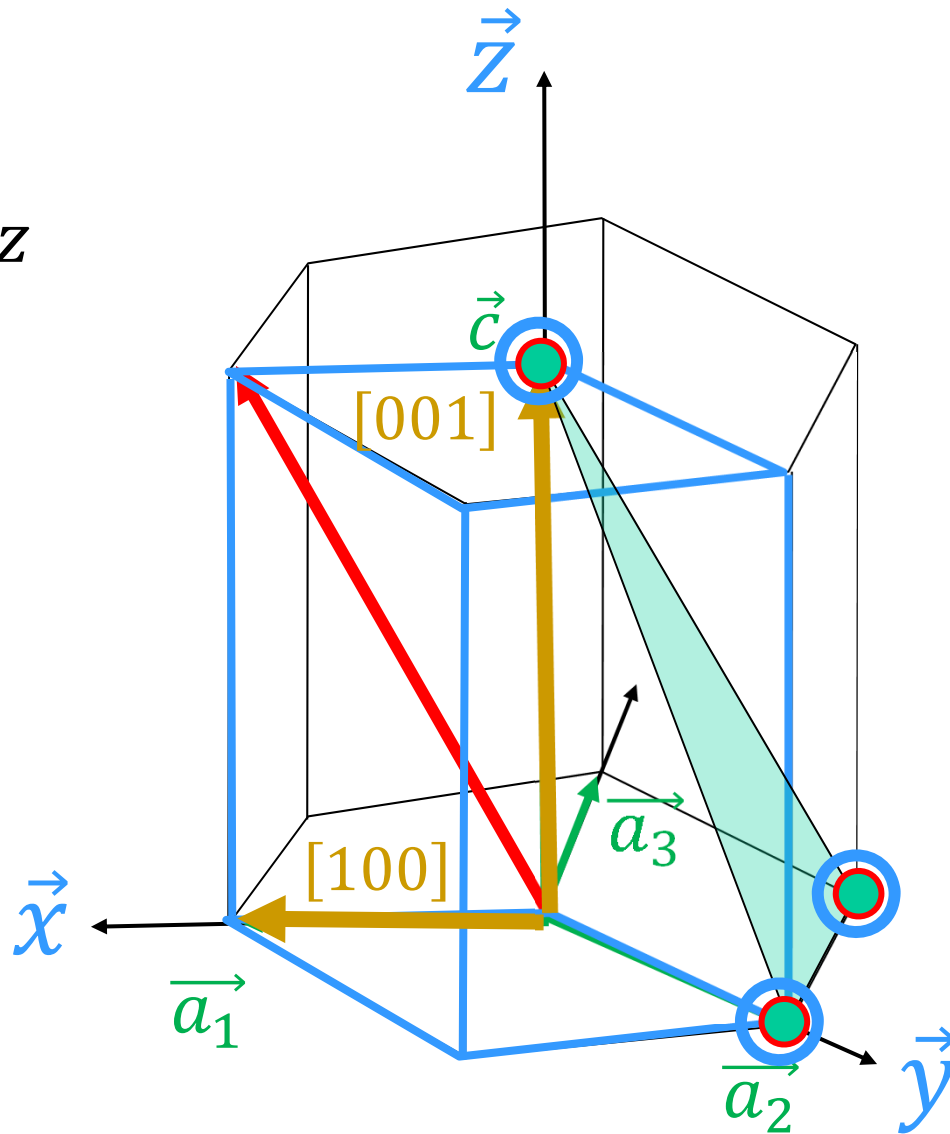
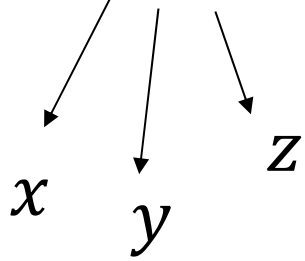


Miller-Bravais index



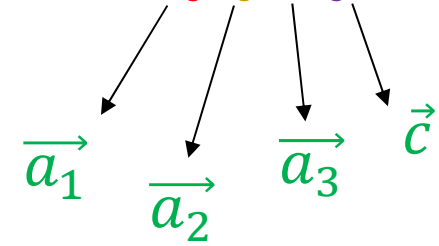
Miller index

$(\bar{1}11)$



Miller-Bravais index

$(\bar{1}101)$



$$u' = u - t = 2u + v$$

$$v' = v - t = 2v + u$$

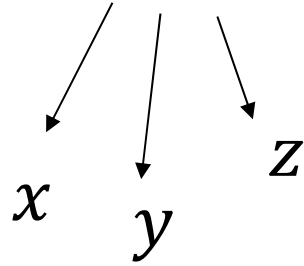
$$w' = w$$

Miller index

$(\bar{1}11)$

Miller index

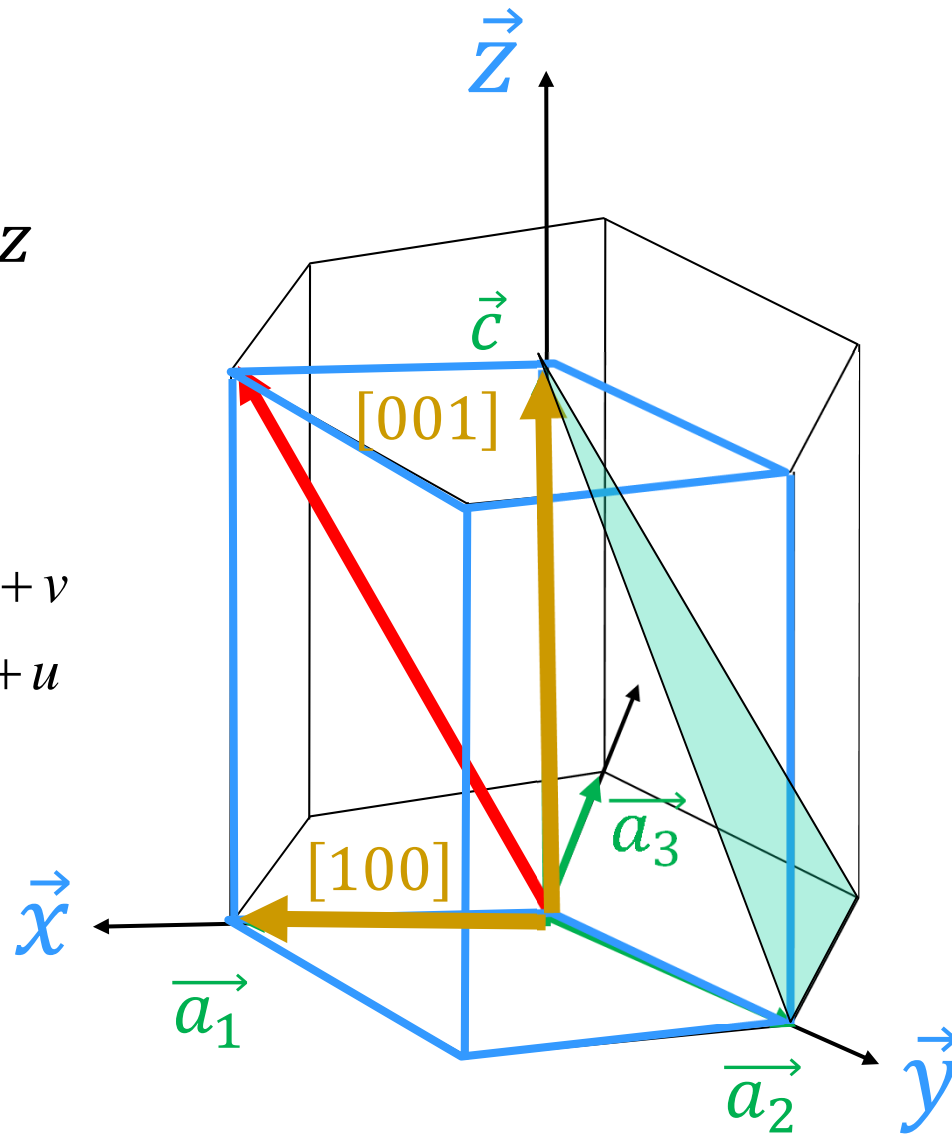
$(\bar{1}11)$



$$u' = u - t = 2u + v$$

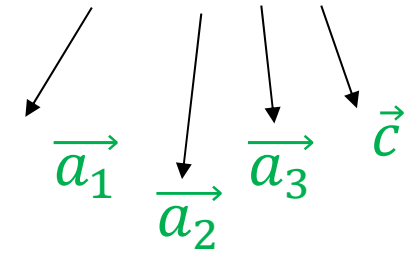
$$v' = v - t = 2v + u$$

$$w' = w$$



Miller-Bravais index

$(\bar{1}101)$



$(10\bar{1}0)$

$$u = \frac{1}{3}(2u' - v')$$

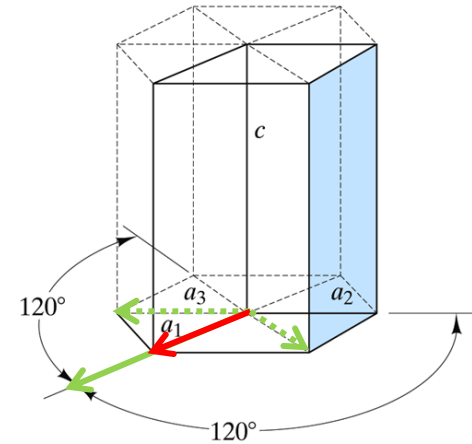
$$v = \frac{1}{3}(2v' - u')$$

$$w = w'$$

Miller-Bravais vs. Miller index system in Hexagonal system

Directions

Miller	Miller-Bravais	Miller	Miller-Bravais
[100]	[2 $\bar{1}$ 10]	[010]	[1 $\bar{2}$ 10]
[110]	[1120]	[110]	
[001]	[0001]		
[011]	[1 $\bar{2}$ 13]	[111]	[11 $\bar{2}$ 3]
[210]	[10 $\bar{1}$ 0]	[120]	[01 $\bar{1}$ 0]
[211]	[10 $\bar{1}$ 1]	[112]	[11 $\bar{2}$ 6]



Conversion of 4 index system (Miller-Bravais) to 3 index (Miller)

$$\vec{t} = u'\vec{a}_1 + v'\vec{a}_2 + w'\vec{c} = u\vec{a}_1 + v\vec{a}_2 + t\vec{a}_3 + w\vec{c}$$

Miller-Bravais to Miller
4 to 3 axis

$$u' = u - t = 2u + v$$

$$v' = v - t = 2v + u$$

$$w' = w$$

Miller to Miller-Bravais
3axis to 4 axis system

$$u = \frac{1}{3}(2u' - v')$$

$$v = \frac{1}{3}(2v' - u')$$

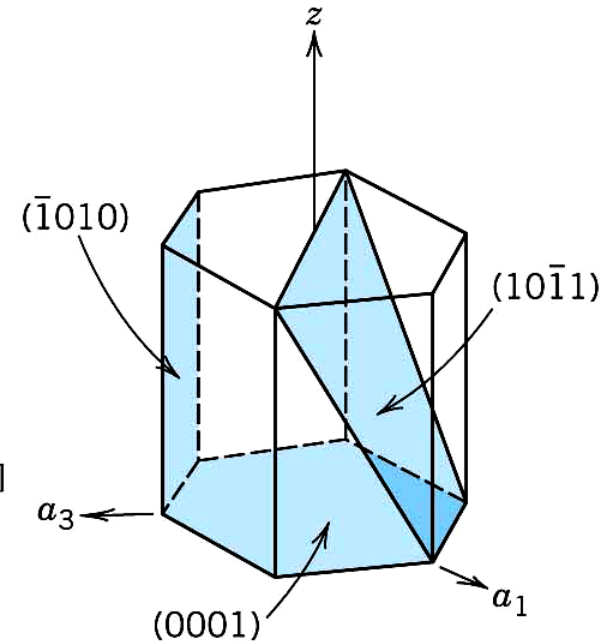
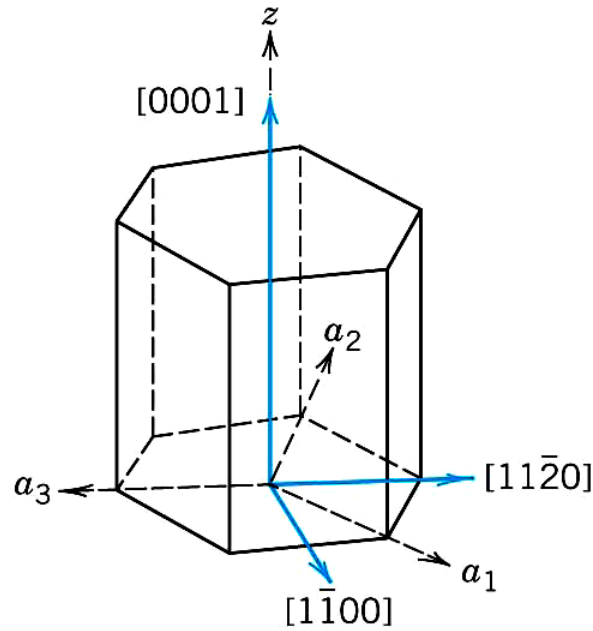
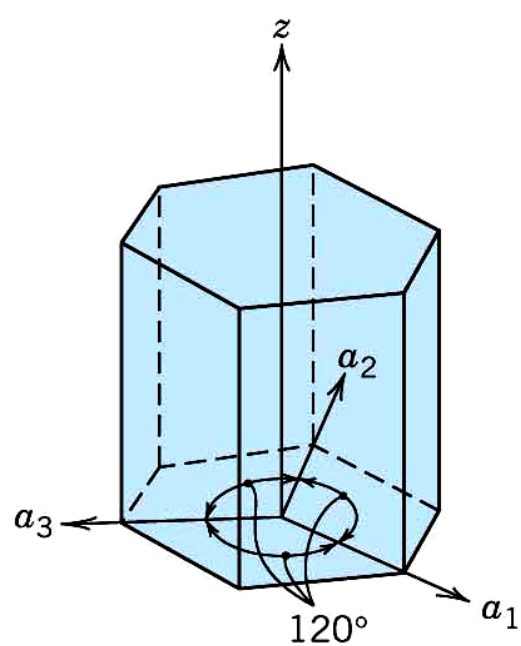
$$w = w'$$

Ex. M [100]
 $u = (1/3)(2*1 - 0) = 2/3$
 $v = (1/3)(2*0 - 1) = -1/3$
 $w = 0$
 $\Rightarrow 1/3[2 \ -1 \ -1 \ 0]$

Ex. M-B [1 0 -1 0]
 $u' = 2*1 + 0 = 2$
 $v' = 2*0 + 1 = 1$
 $w' = 0$
 $\Rightarrow [2 \ 1 \ 0]$

Hexagonal Crystal

- Miller-Bravais scheme



$$[uvw]$$

$$t = -(u + v)$$

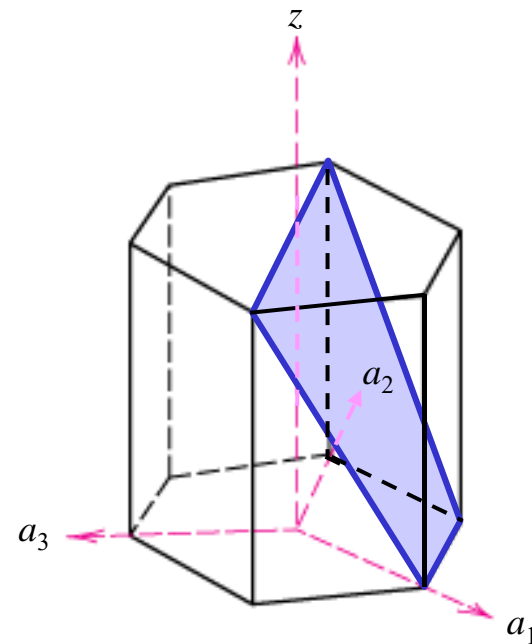
$$(hkil)$$

$$i = -(h + k)$$

Crystallographic Planes (HCP)

- In hexagonal unit cells the same idea is used

<u>example</u>	a_1	a_2	a_3	c
1. Intercepts	1	∞	-1	1
2. Reciprocals	1	$1/\infty$	-1	1
	1	0	-1	1
3. Reduction	1	0	-1	1
4. Miller-Bravais Indices				
				$(10\bar{1}1)$

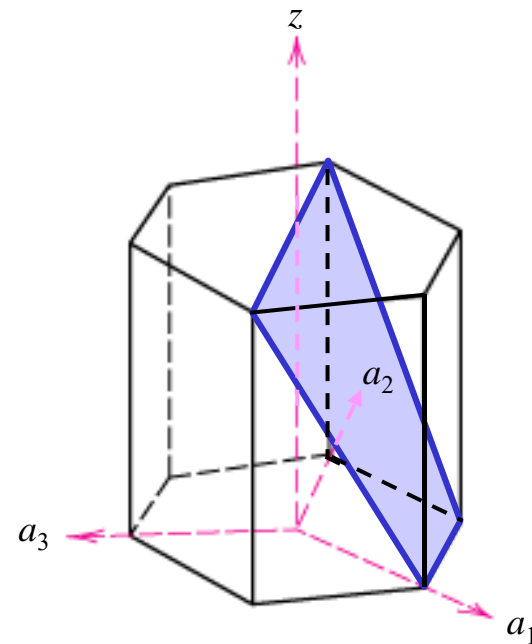


Adapted from Fig. 3.8(a), Callister 7e.

Crystallographic Planes (HCP)

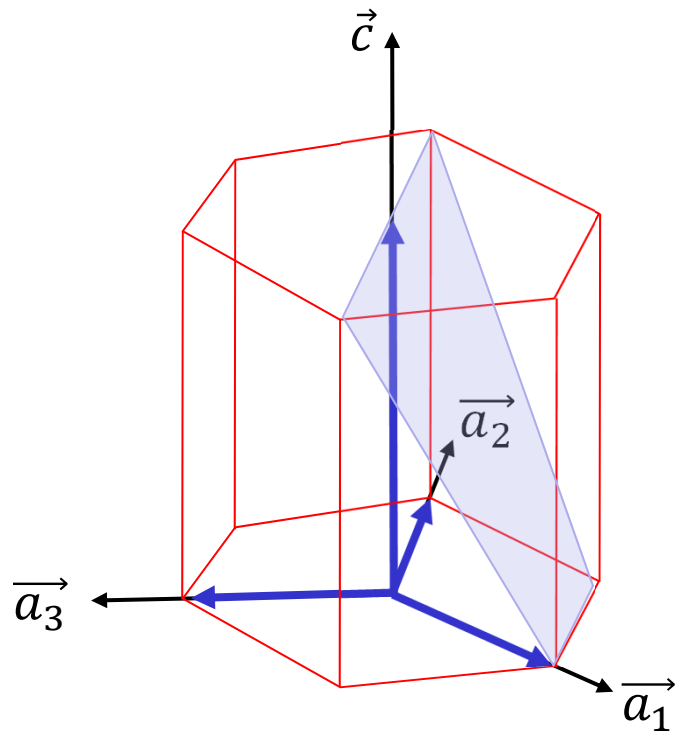
- In hexagonal unit cells the same idea is used

<u>example</u>	a_1	a_2	a_3	c
1. Intercepts	1	∞	-1	1
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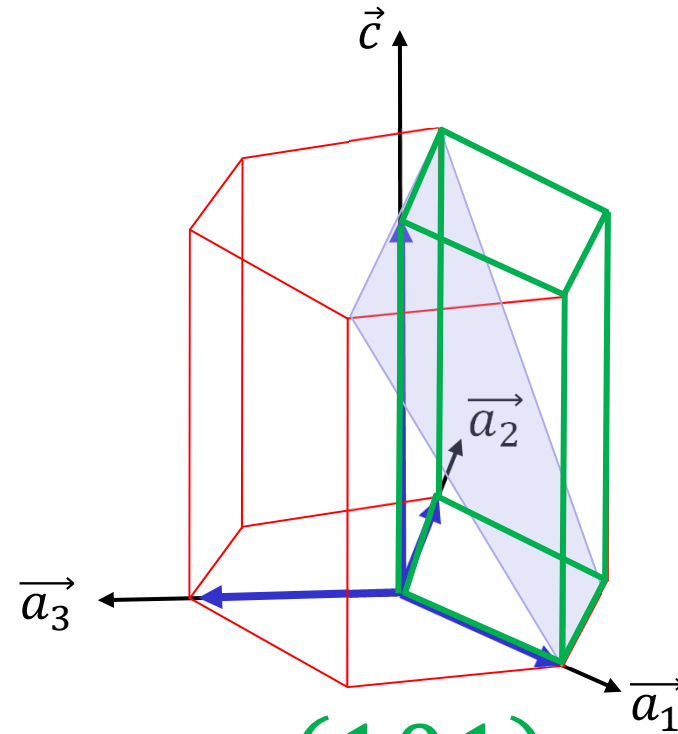


Adapted from Fig. 3.8(a), Callister 7e.

Miller-Bravais index



Miller index



$(10\bar{1}1)$

(101)

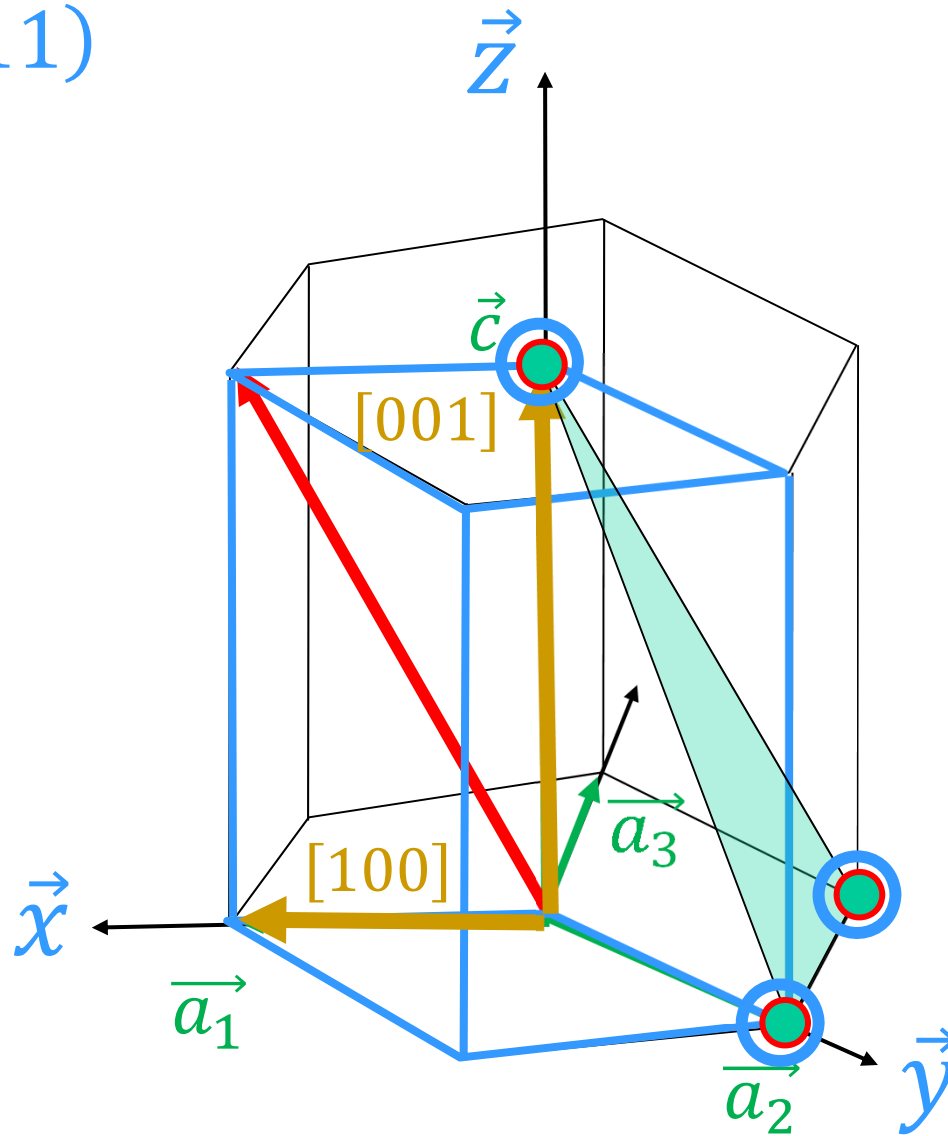
Inverse of 1 = 1
Position at $\vec{a}_1 = 1$

Inverse of 1 = 1
Position at $\vec{c} = 1$

Does not
Meet with \vec{a}_2

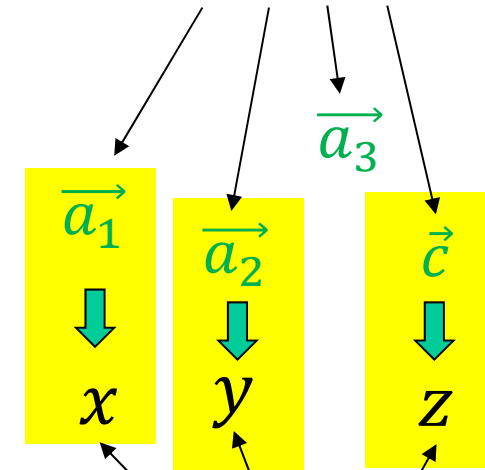
Miller index

$(\bar{1}11)$

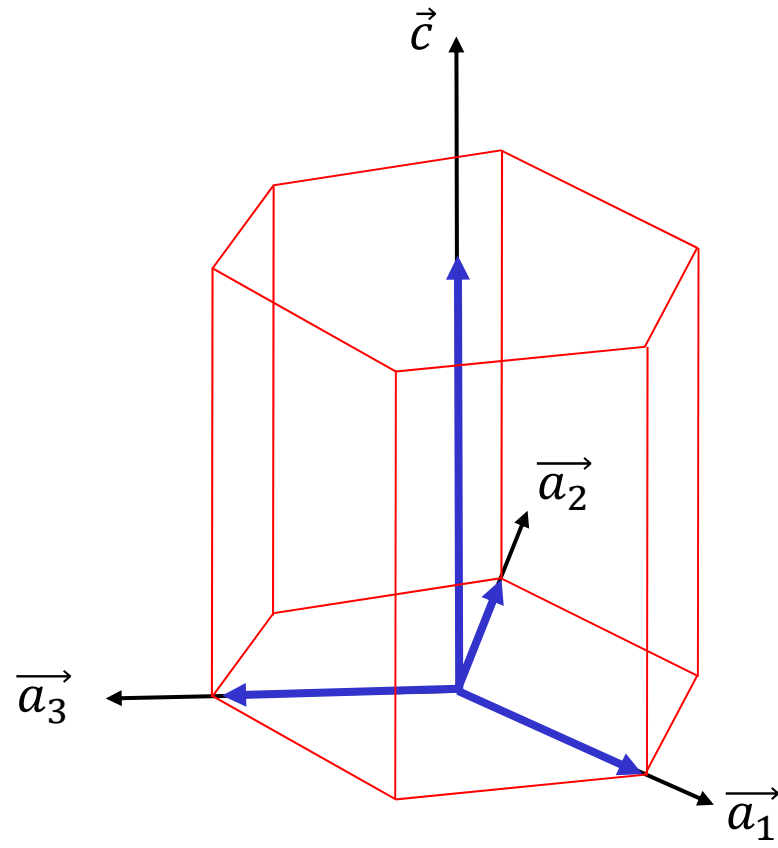


Miller-Bravais index

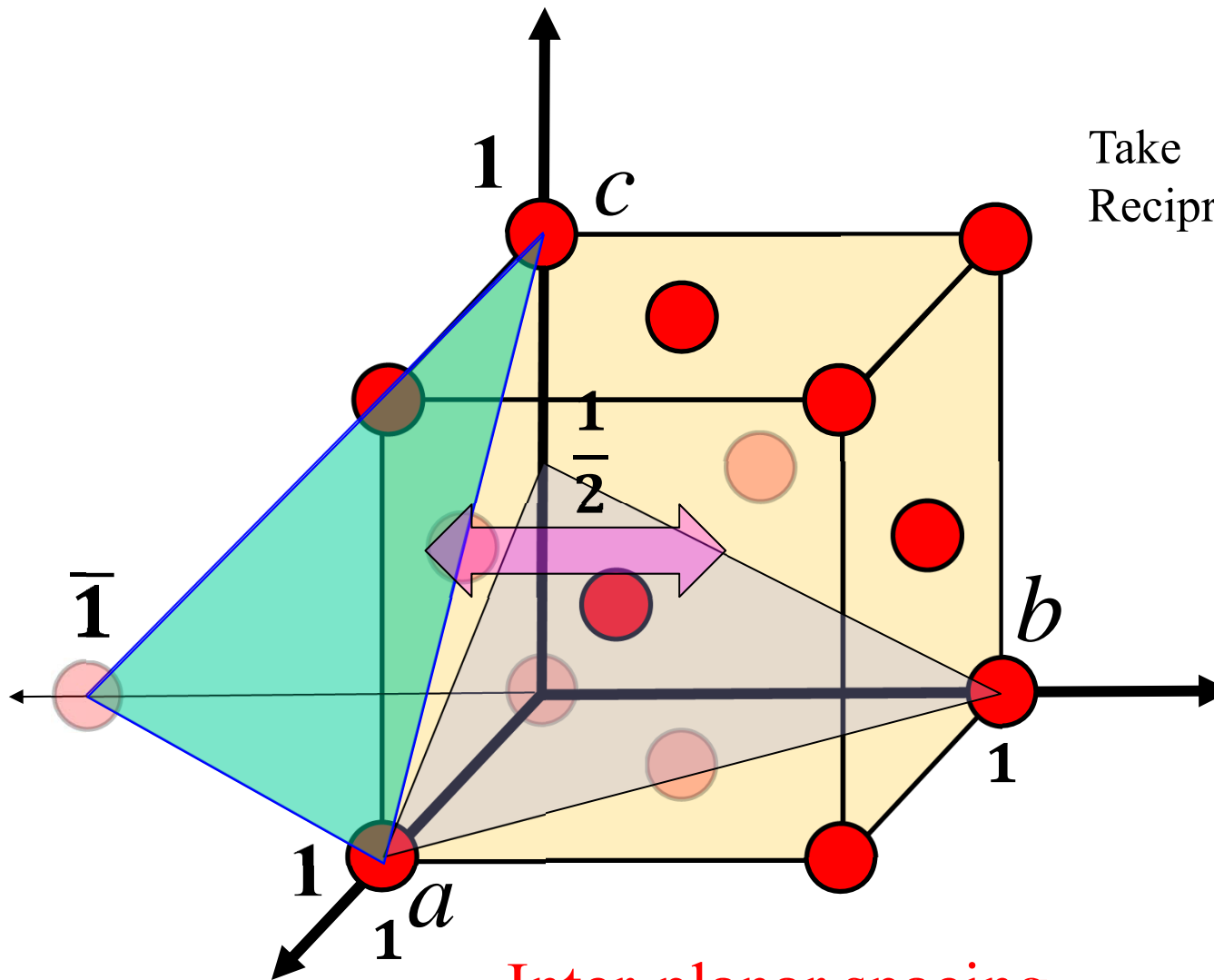
$(\bar{1}101)$



$(\bar{1}11)$
Miller index



Schematic view of planes

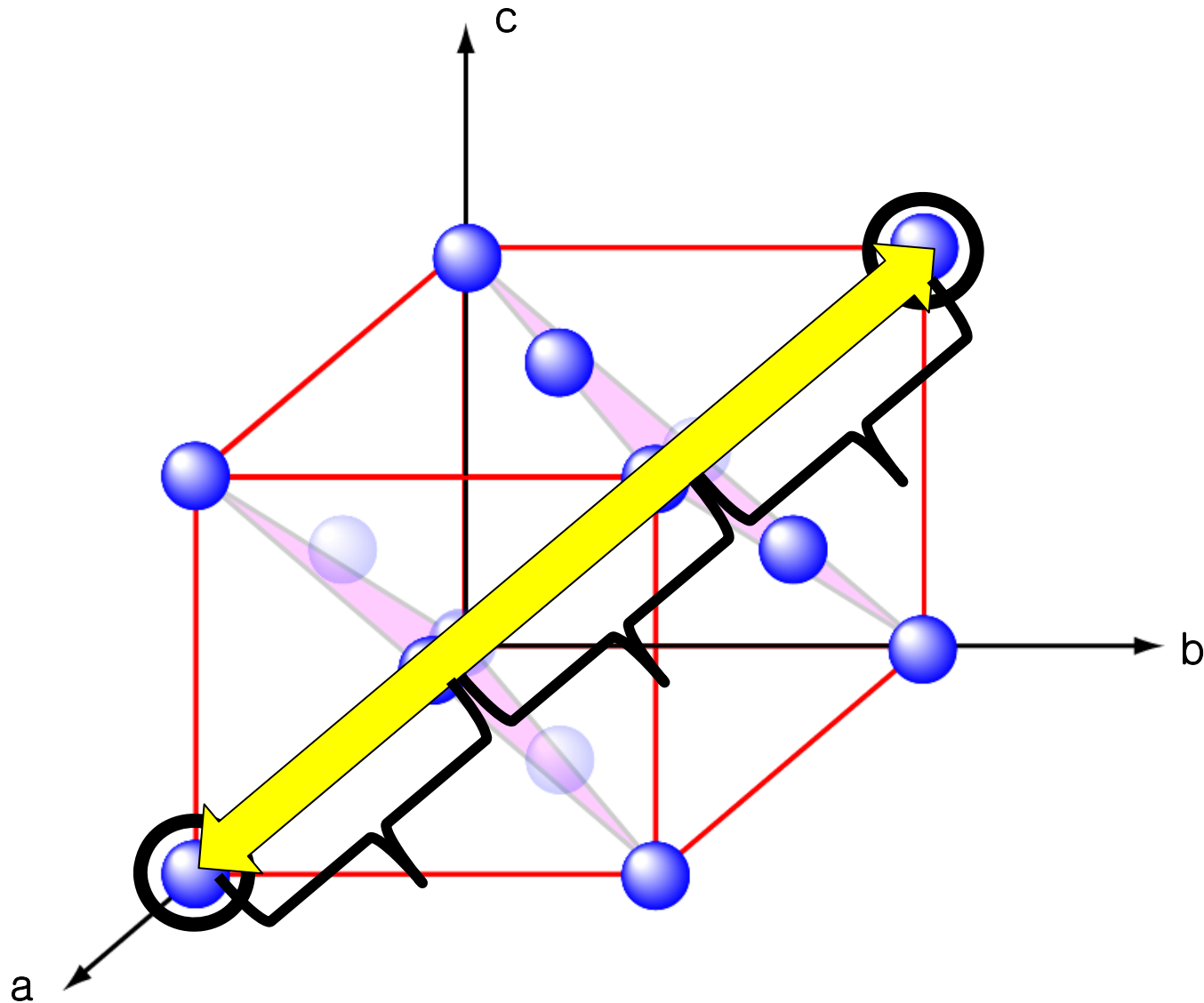


Inter-planar spacing

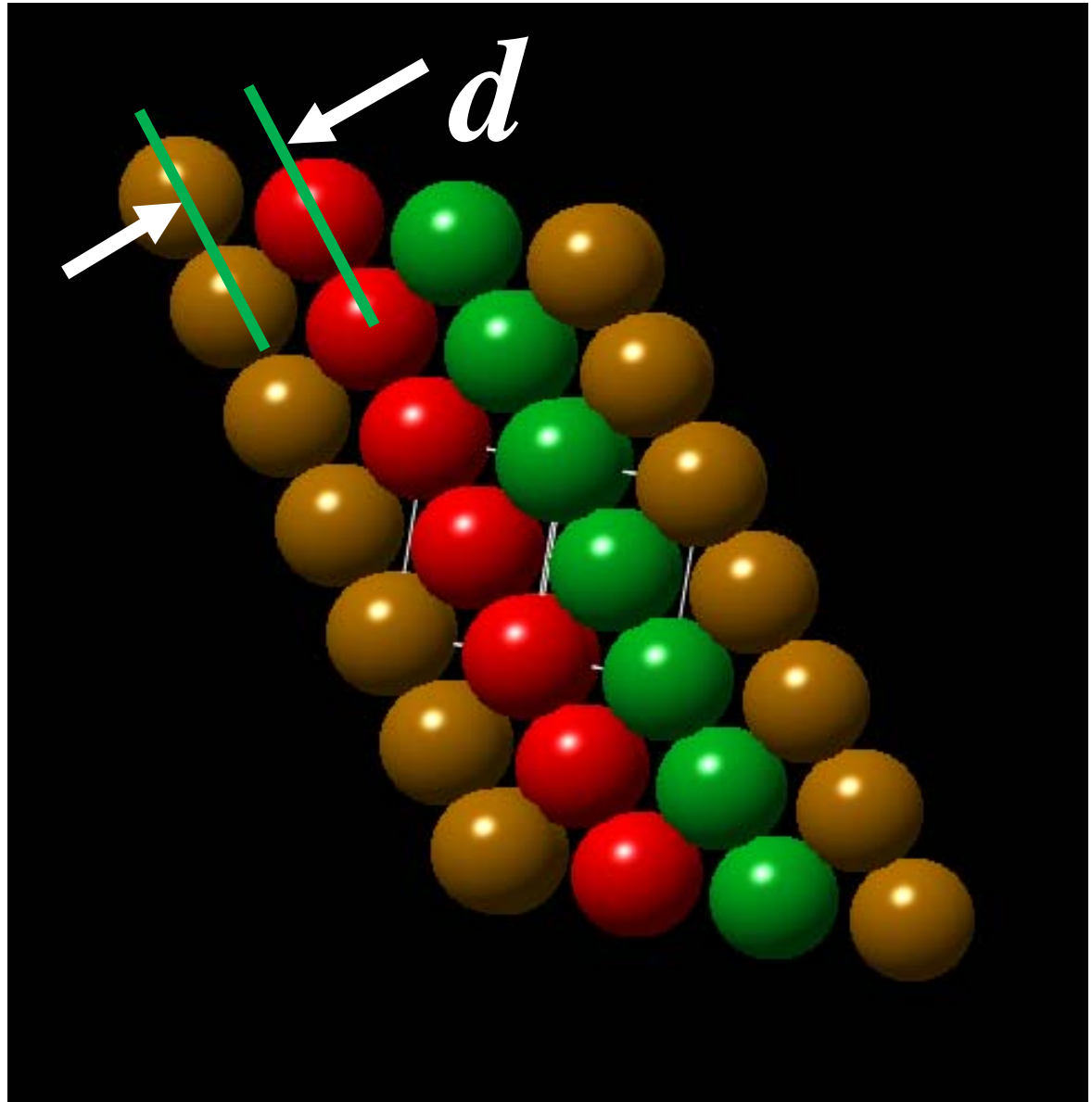
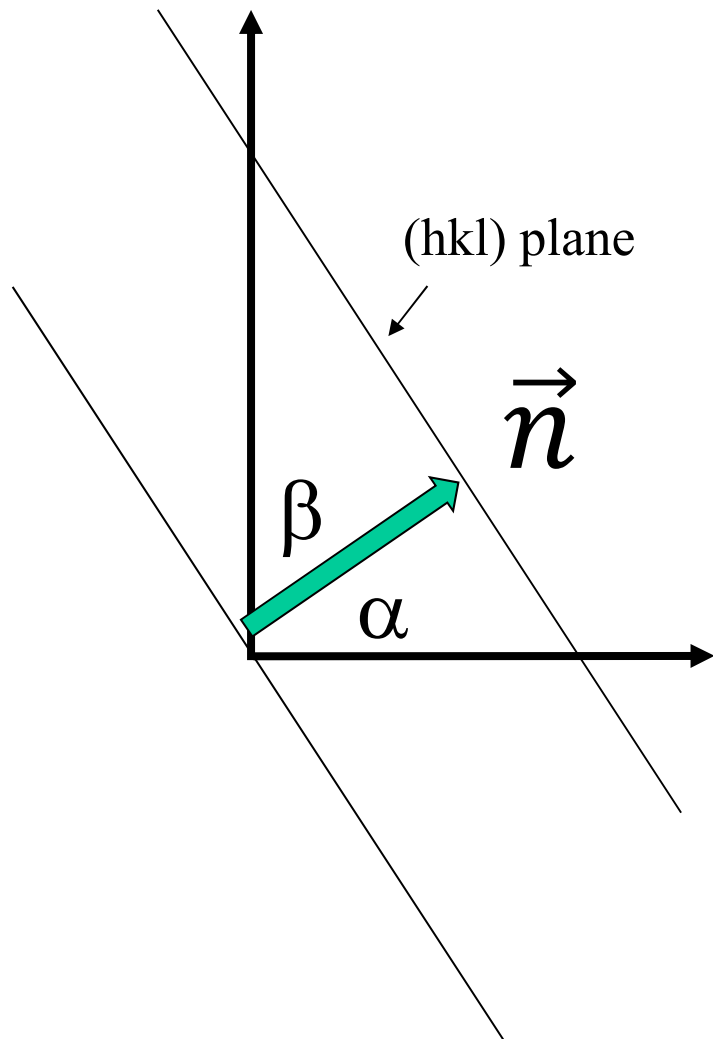
Take
Reciprocal $\Rightarrow 1 \ 1 \ \frac{1}{2}$

$(1\bar{1}1)$

Schematic view of $(\bar{1}11)$ plane



Inter-planar distance (면간거리)



Interplanar spacing of the (hkl) plane

The value of d which characterizes the distance between adjacent planes in the set of planes with Miller indices (hkl) is given by the following relations. The cell edges and the angles are a, b, c and α, β, γ .

$$\text{Cubic :} \quad \frac{1}{d^2} = \frac{h^2 + k^2 + l^2}{a^2}$$

$$\text{Tetragonal :} \quad \frac{1}{d^2} = \frac{h^2 + k^2}{a^2} + \frac{l^2}{c^2}$$

$$\text{Orthorhombic :} \quad \frac{1}{d^2} = \frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2}$$

$$\text{Hexagonal :} \quad \frac{1}{d^2} = \frac{4}{3} \left(\frac{h^2 + hk + k^2}{a^2} \right) + \frac{l^2}{c^2}$$

$$\text{Rhombohedral :} \quad \frac{1}{d^2} = \frac{1}{\sin^2 \beta} \left(\frac{h^2}{a^2} + \frac{k^2 \sin^2 \beta}{b^2} + \frac{l^2}{c^2} - \frac{2hl \cos \beta}{ac} \right)$$

$$\text{Monoclinic :} \quad \frac{1}{d^2} = \frac{(h^2 + k^2 + l^2) \sin^2 \alpha + 2(hk + kl + hl)(\cos^2 \alpha - \cos \alpha)}{a^2(1 - 3\cos^2 \alpha + 2\cos^3 \alpha)}$$

$$\text{Triclinic :} \quad \frac{1}{d^2} = \frac{1}{V^2} (S_{11}h^2 + S_{22}k^2 + S_{33}l^2 + 2S_{12}hk + 2S_{23}kl + 2S_{31}hl)$$

$$\text{Where :} \quad V^2 = a^2b^2c^3(1 - \cos^2 \alpha - \cos^2 \beta - \cos^2 \gamma + 2\cos \alpha \cos \beta \cos \gamma)$$

$$S_{11} = b^2c^2 \sin^2 \alpha$$

$$S_{22} = a^2c^2 \sin^2 \beta$$

$$S_{33} = a^2b^2 \sin^2 \gamma$$

$$S_{12} = abc^2(\cos \alpha \cos \beta - \cos \gamma)$$

$$S_{23} = a^2bc(\cos \beta \cos \gamma - \cos \alpha)$$

$$S_{31} = ab^2c(\cos \gamma \cos \alpha - \cos \beta)$$

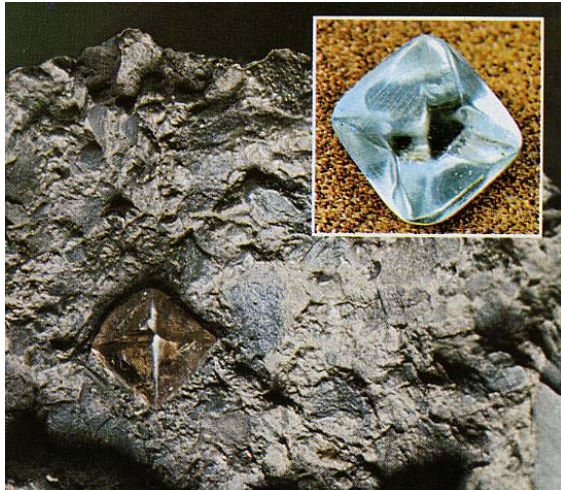
III. Crystalline and Noncrystalline Materials

CRYSTALS AS BUILDING BLOCKS

- *Some* engineering applications require single crystals:

--diamond single crystals

Natural and artificial



(Courtesy Martin Deakins, GE Superabrasives, Worthington, OH. Used with permission.)

--turbine blades

Fig. 8.30(c), *Callister 6e*.
(Fig. 8.30(c) courtesy of Pratt and Whitney).



- Crystal properties reveal features of atomic structure.

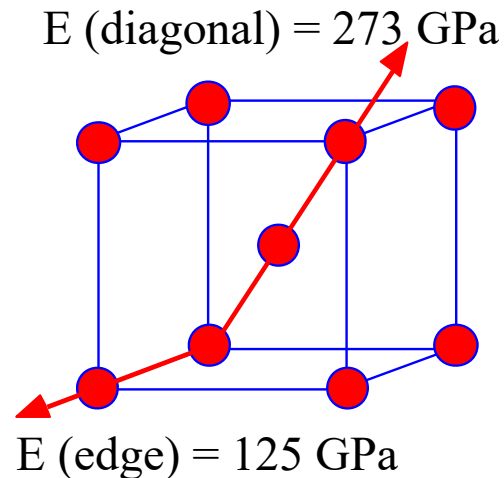
--Ex: Certain crystal planes in quartz fracture more easily than others.



(Courtesy P.M. Anderson)

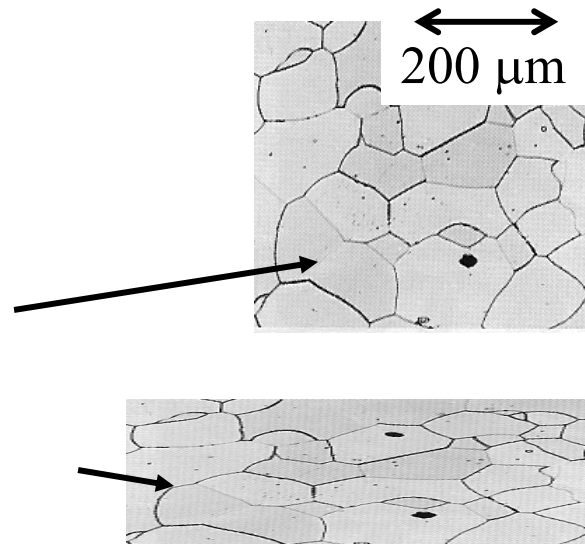
Single vs Polycrystals

- Single Crystals
 - Properties vary with direction: **anisotropic**.
 - Example: the modulus of elasticity (E) in BCC iron:



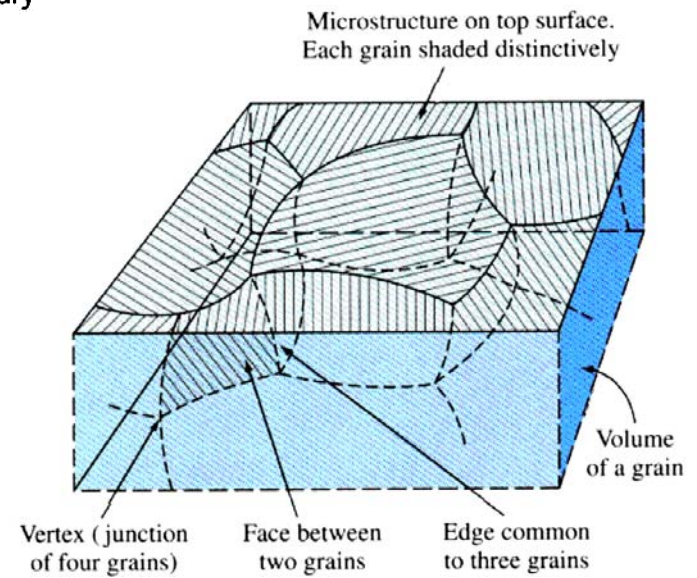
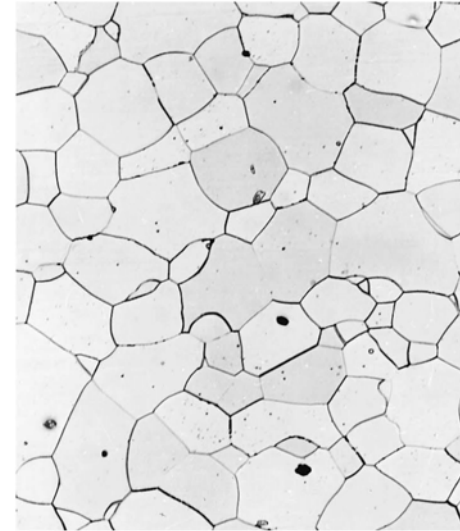
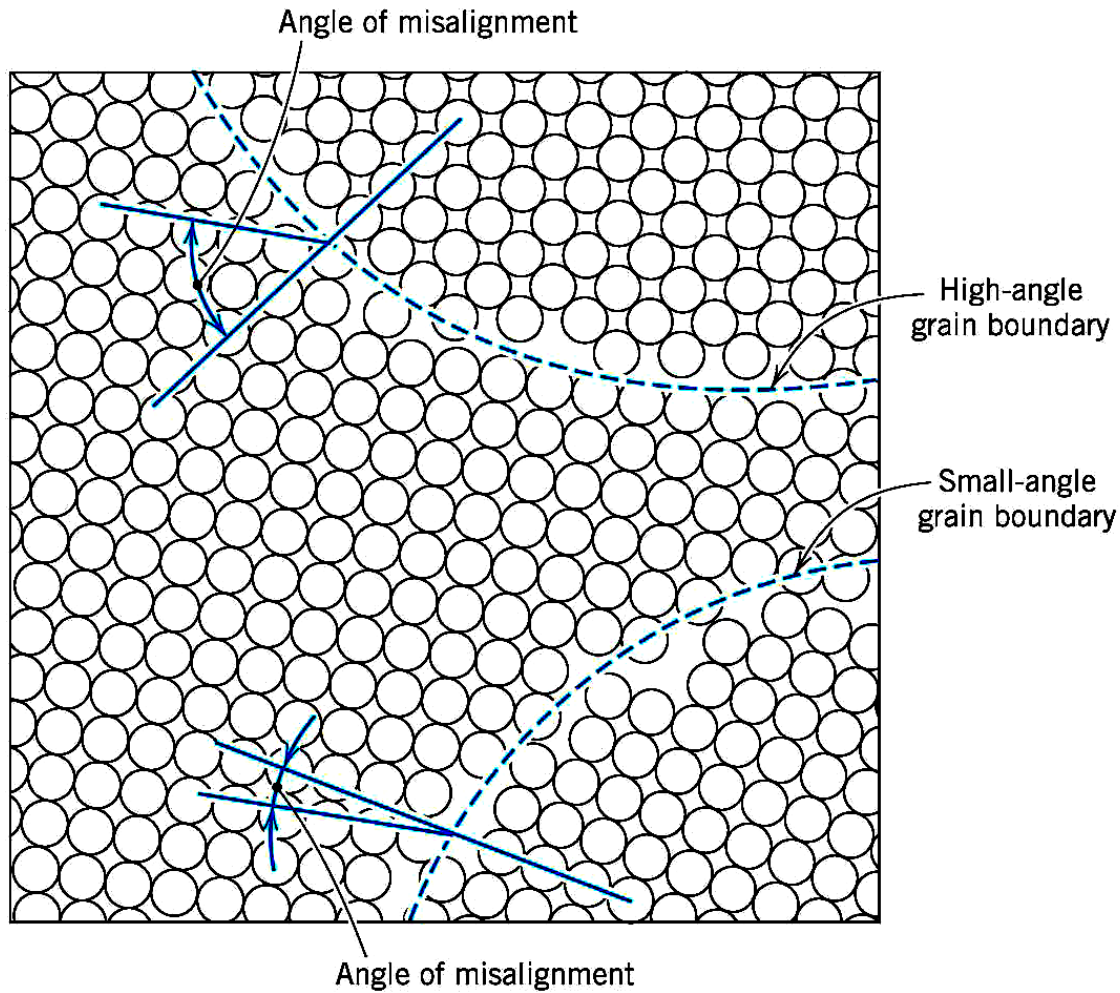
Data from Table 3.3, *Callister 7e*.
(Source of data is R.W. Hertzberg, *Deformation and Fracture Mechanics of Engineering Materials*, 3rd ed., John Wiley and Sons, 1989.)

- Polycrystals
 - Properties may/may not vary with direction.
 - If grains are randomly oriented: **isotropic**.
($E_{\text{poly iron}} = 210$ GPa)
 - If grains are **textured**, anisotropic.



Adapted from Fig. 4.14(b), *Callister 7e*.
(Fig. 4.14(b) is courtesy of L.C. Smith and C. Brady, the National Bureau of Standards, Washington, DC [now the National Institute of Standards and Technology, Gaithersburg, MD].)

Grain Boundaries



Polycrystals

- *Most* engineering materials are polycrystals.



Anisotropic

Adapted from Fig. K, color inset pages of *Callister 5e*. (Fig. K is courtesy of Paul E. Danielson, Teledyne Wah Chang Albany)

Isotropic

- Nb-Hf-W plate with an electron beam weld.
- Each "grain" is a single crystal.
- If grains are randomly oriented, overall component properties are not directional.
- Grain sizes typ. range from 1 nm to 2 cm (i.e., from a few to millions of atomic layers).

Polymorphism

- Two or more distinct crystal structures for the same material (allotropy/polymorphism)

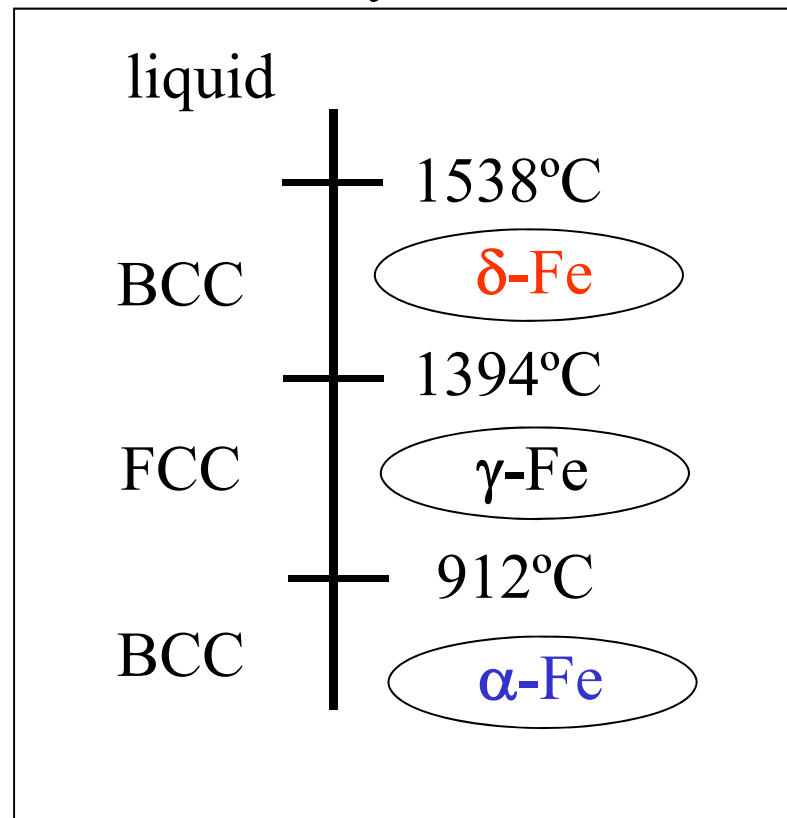
titanium

α , β -Ti

carbon

diamond, graphite

iron system



DEMO: HEATING AND COOLING OF AN IRON WIRE

- Demonstrates "polymorphism" ← The same atoms can have more than one crystal structure.

