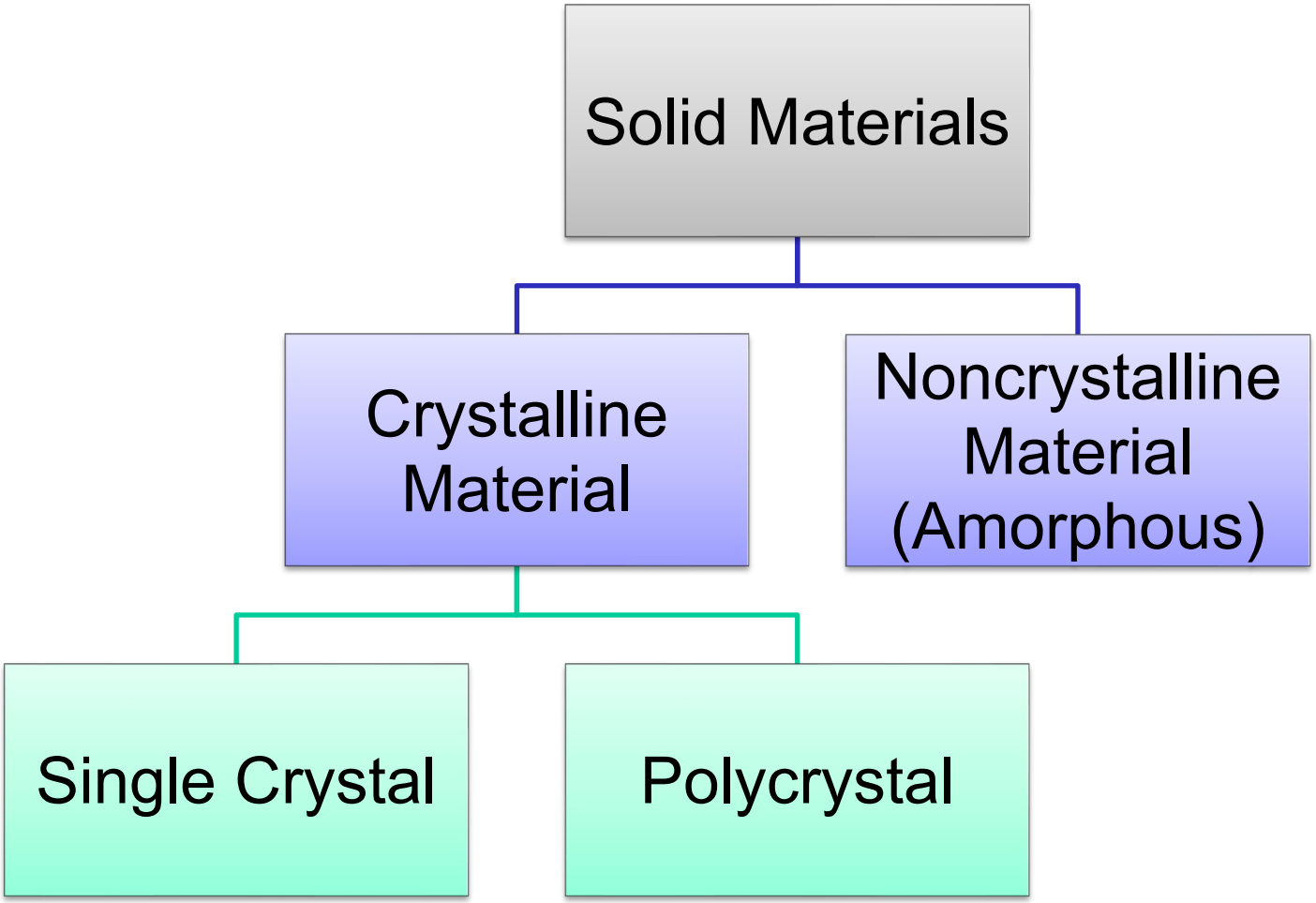
Chapter 3: Fundamentals of Crystallography

ISSUES TO ADDRESS...

- What is the difference in atomic arrangement between crystalline and noncrystalline solids?
- How are crystallographic directions and planes named?
- Under what circumstances does a material property vary with the measurement direction?

Fundamental Concept: Classification of Solid Materials

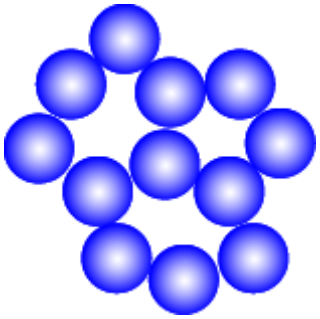


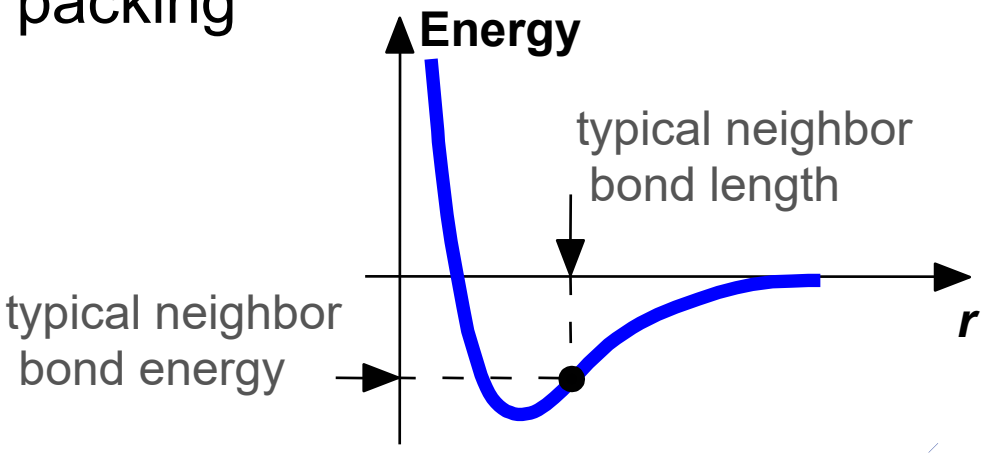
Fundamental concept: Crystalline material

- Crystalline material- atoms, molecules or ion packed in a regularly ordered, repeating pattern, extending in 3 spatial dimension.
- Properties of crystalline materials depend on the crystal structure
- Crystal structure
  - **is a unique arrangement of atoms in a crystal.**
  - **composed of a unit cell**

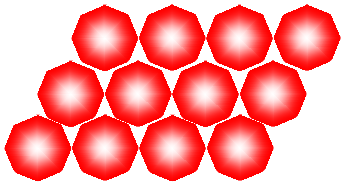
Energy and Packing

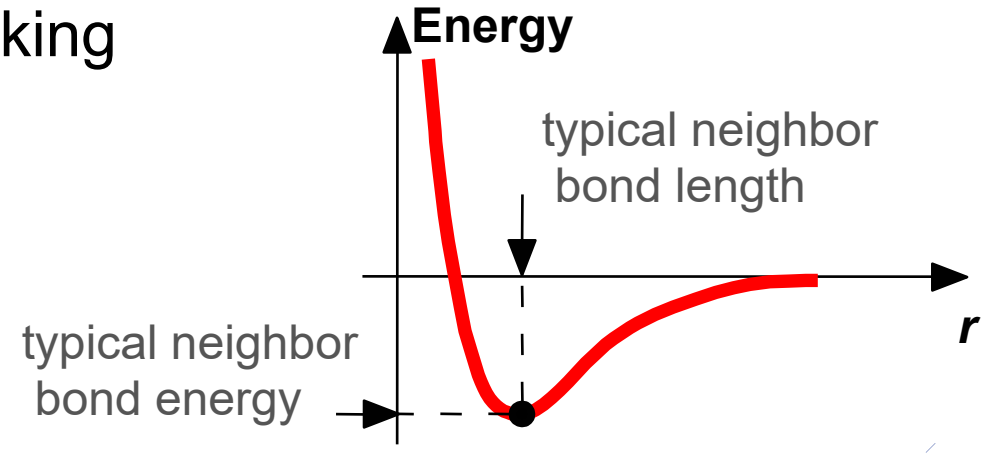
- Non dense, random packing





- Dense, ordered packing



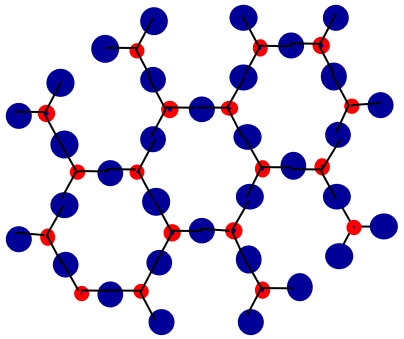


Dense, ordered packed structures tend to have lower energies.

Materials and Packing

Crystalline materials...

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



crystalline SiO_2

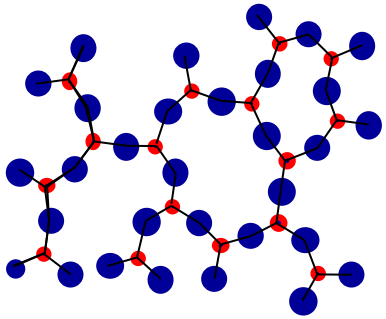
Adapted from Fig. 3.11(a), *Callister & Rethwisch 9e.*

• Si • Oxygen

Noncrystalline materials...

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

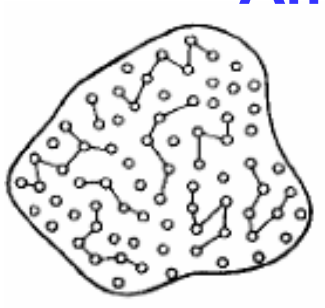
"Amorphous" = Noncrystalline

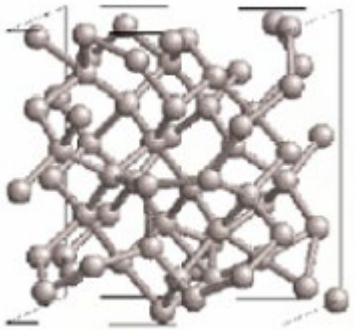


noncrystalline SiO_2

Adapted from Fig. 3.11(b), *Callister & Rethwisch 9e.*

Amorphous



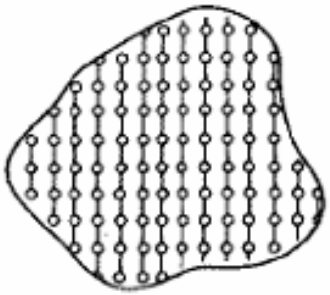


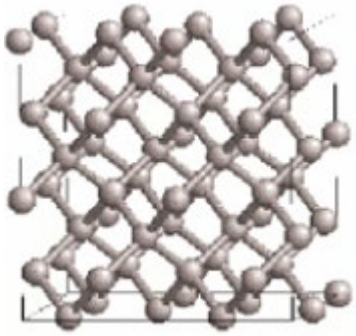
•No recognizable long-range order

•Atoms are disordered

•No lattice

Crystal





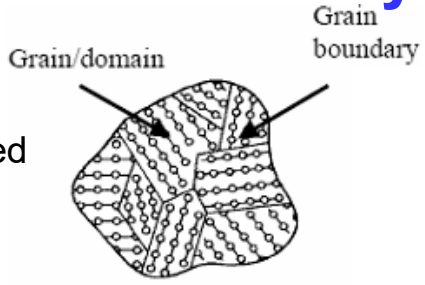
•Entire solid is made up of atoms in an orderly array

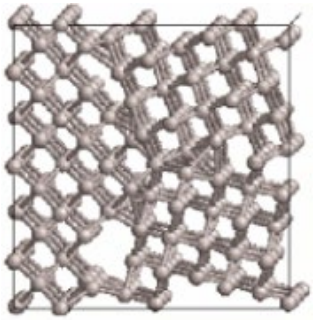
•All atoms arranged on a common lattice

Polycrystalline

•Completely ordered

•In segments

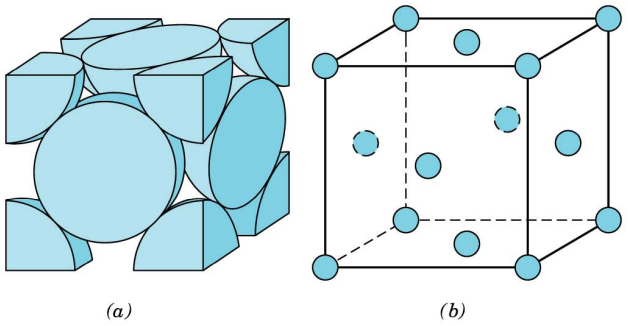




•Different lattice orientation for each grain

SOME DEFINITIONS …

- **Lattice**: 3D array of regularly spaced points
- **Crystalline material:** atoms situated in a repeating 3D periodic array over large atomic distances
- **Amorphous material:** material with no such order
- **Hard sphere representation:** atoms denoted by hard, touching spheres
- Reduced sphere representation
- **Unit cell:** basic building block unit (such as a flooring tile) that repeats in space to create the crystal structure



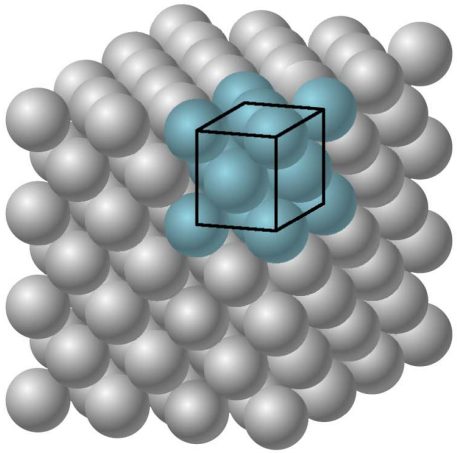


FIGURE 3.1 For the face-centered cubic crystal structure: (*a*) a hard sphere unit cell representation, (*b*) a reduced-sphere unit cell, and (*c*) an aggregate of many atoms. (Figure *c* adapted from W. G. Moffatt, G. W. Pearsall, and J. Wulff, *The Structure and Properties of Materials*, Vol. I, *Structure*, p. 51. Copyright © 1964 by John Wiley & Sons, New York. Reprinted by permission of John Wiley & Sons, Inc.)

CRYSTAL SYSTEMS

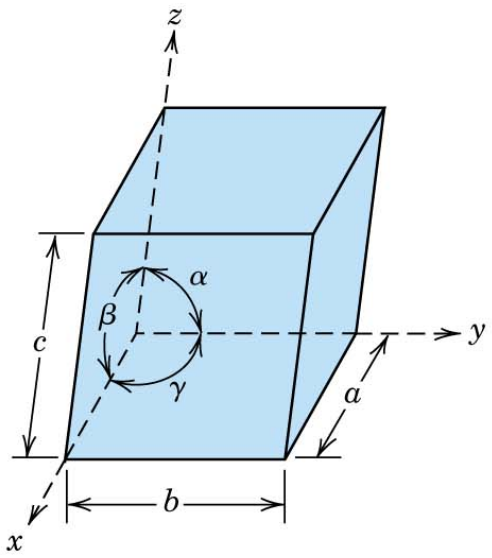
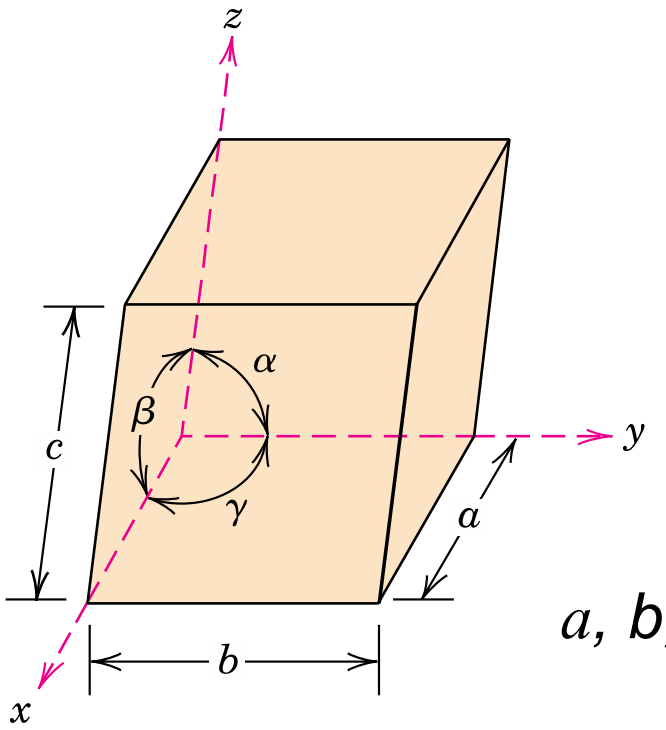


FIGURE 3.4 A unit cell with x, y, and z coordinate axes, showing axial lengths (a, b, and c) and interaxial angles (α, β, and γ).

- Based on shape of unit cell ignoring actual atomic locations
- Unit cell = 3-dimensional unit that repeats in space
- Unit cell geometry completely specified by *a, b, c* & α, β, γ ***(lattice parameters** or **lattice constants**)*
- Seven possible combinations of *a, b, c* & α, β, γ, resulting in seven crystal systems

Crystal Systems

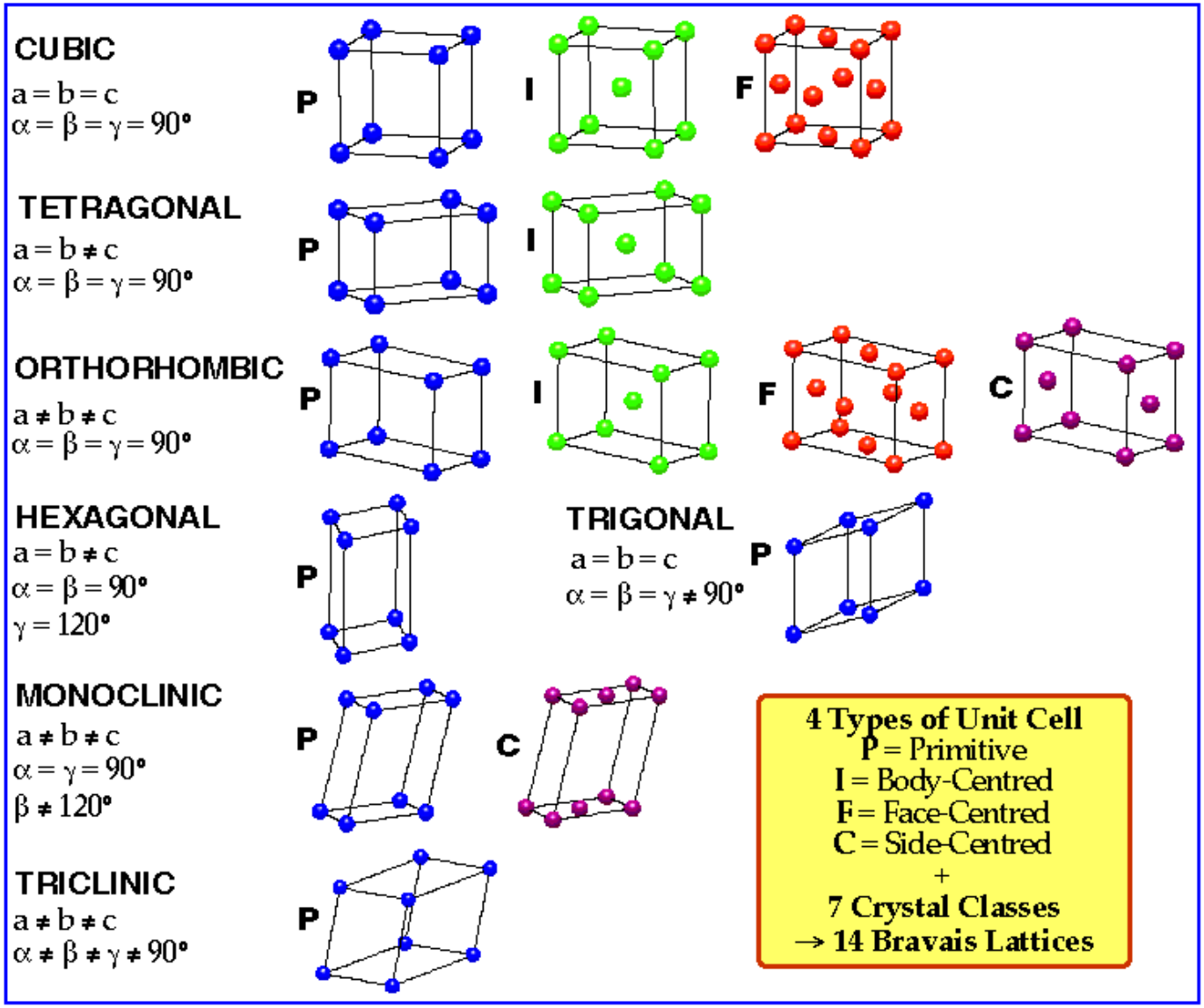
Unit cell: smallest repetitive volume which contains the complete lattice pattern of a crystal.



7 crystal systems

a, *b*, and *c* are the lattice constants

CRYSTAL SYSTEMS



CRYSTALLOGRAPHIC POINTS, DIRECTIONS & PLANES

- In crystalline materials, often necessary to specify points, directions and planes within unit cell and in crystal lattice
- Three numbers (or indices) used to designate points, directions (lines) or planes, based on basic geometric notions
- The three indices are determined by placing the origin at one of the corners of the unit cell, and the coordinate axes along the unit cell edges

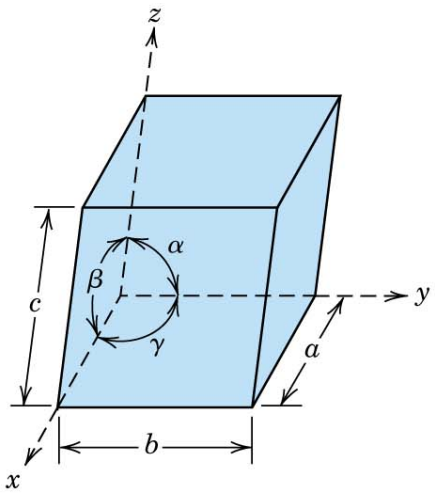
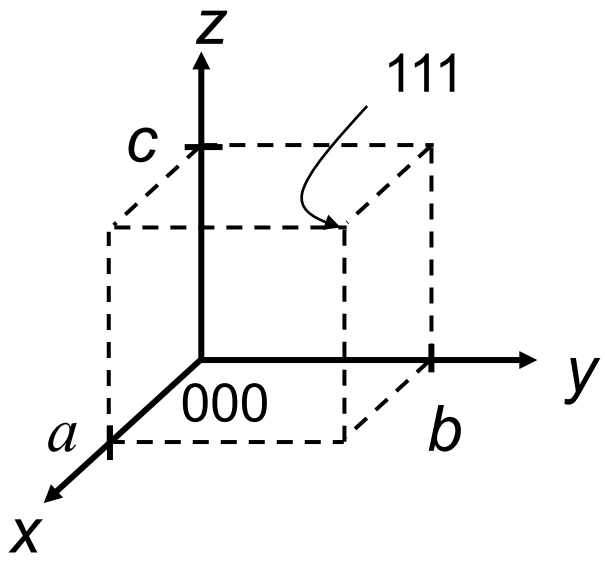


FIGURE 3.4 A unit cell with x, y, and z coordinate axes, showing axial lengths (a, b, and c) and interaxial angles (α, β, and γ).

Point Coordinates



Point coordinates for unit cell center are

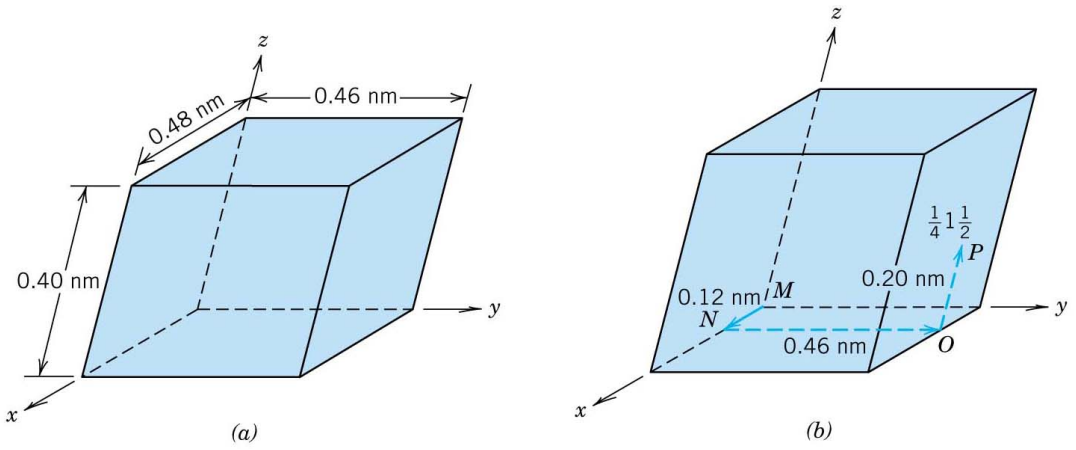
$a/2, b/2, c/2$ ½ ½ ½

Point coordinates for unit cell corner are 111

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

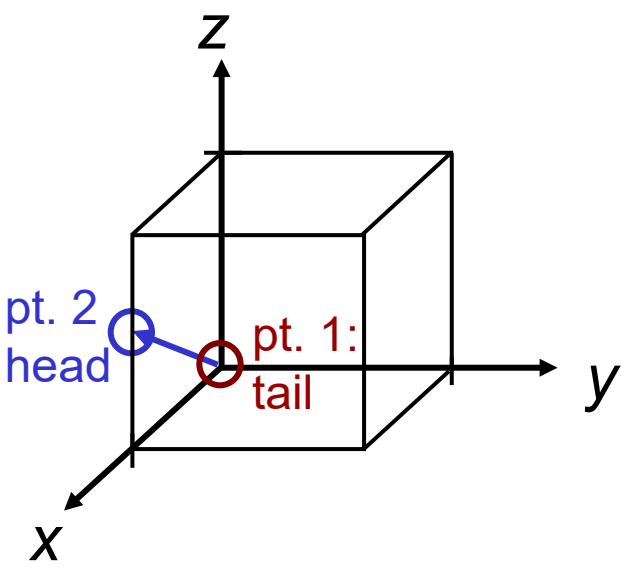
EXAMPLE: POINT COORDINATES

- Locate the point (1/4 1 ½)



- Specify point coordinates for all atom positions for a BCC unit cell
  - Answer: 0 0 0, 1 0 0, 1 1 0, 0 1 0, ½ ½ ½, 0 0 1, 1 0 1, 1 1 1, 0 1 1

Crystallographic Directions



Algorithm

1. Determine coordinates of vector tail, pt. 1: x_1, y_1, & z_1; and vector head, pt. 2: x_2, y_2, & z_2.
2. Tail point coordinates subtracted from head point coordinates.
3. Normalize coordinate differences in terms of lattice parameters a, b, and c:

$$\frac{x_2 - x_1}{a} \quad \frac{y_2 - y_1}{b} \quad \frac{z_2 - z_1}{c}$$

4. Adjust to smallest integer values
5. Enclose in square brackets, no commas

[*uvw*]

ex:

pt. 1 $x_1 = 0$, $y_1 = 0$, $z_1 = 0$

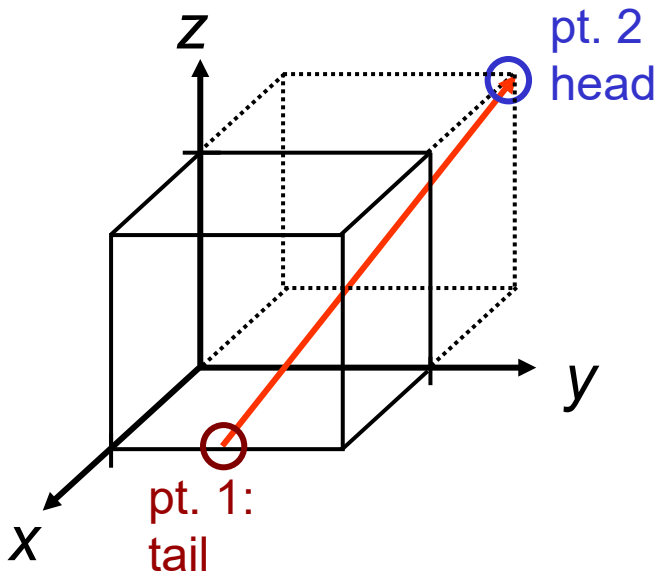
pt. 2 $x_2 = a$, $y_2 = 0$, $z_2 = c/2$

$$\frac{a-0}{a} \quad \frac{0-0}{b} \quad \frac{c/2-0}{c}$$

=> 1, 0, 1/2 => 2, 0, 1

=> [201]

Crystallographic Directions



Example 2:

pt. 1 $x_1 = a$, $y_1 = b/2$, $z_1 = 0$

pt. 2 $x_2 = -a$, $y_2 = b$, $z_2 = c$

$$\frac{-a-a}{a} \quad \frac{b-b/2}{b} \quad \frac{c-0}{c}$$

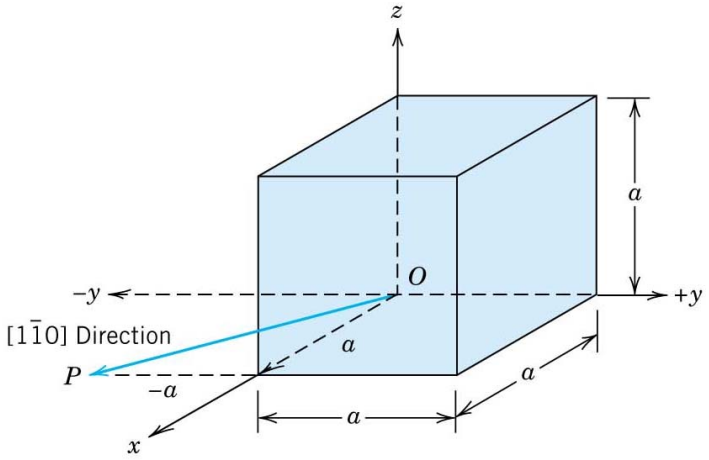
=> -2, 1/2, 1

Multiplying by 2 to eliminate the fraction

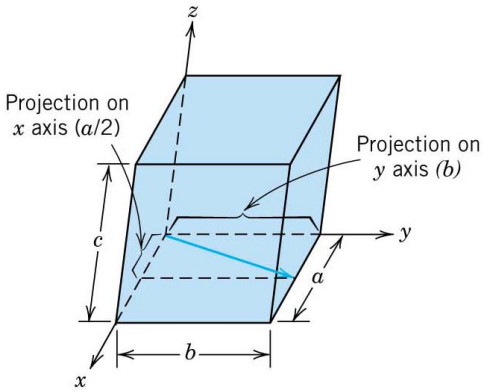
-4, 1, 2 => $[\bar{4}12]$ where the overbar represents a negative index

EXAMPLES: DIRECTIONS

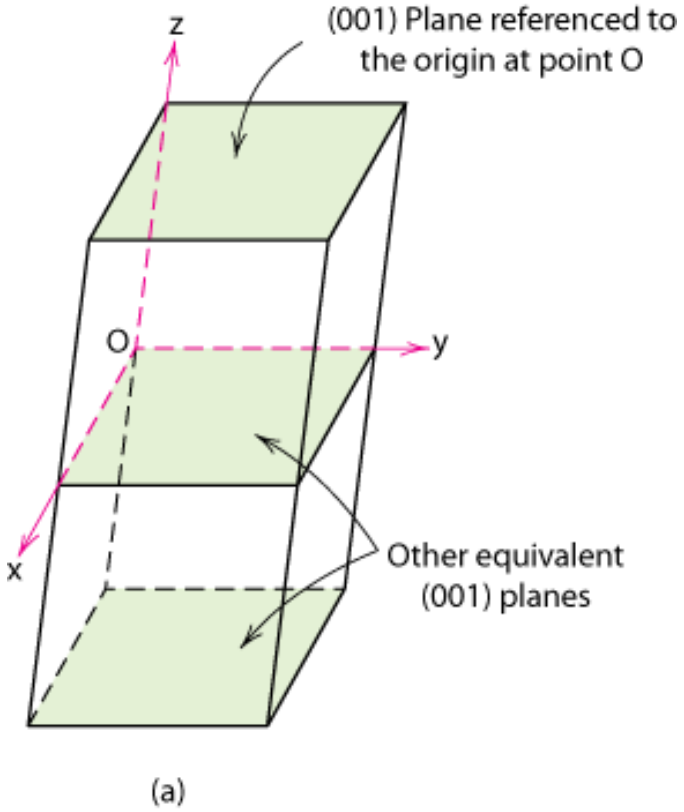
- Draw a $[1\bar{1}0]$ direction within a cubic unit cell

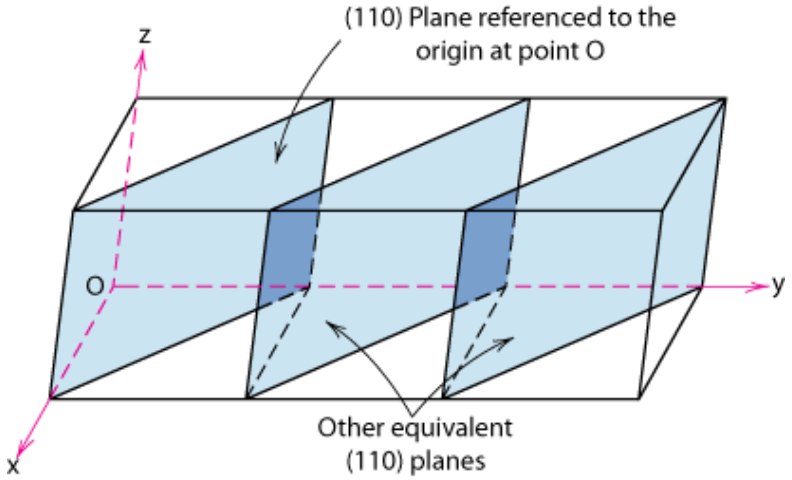


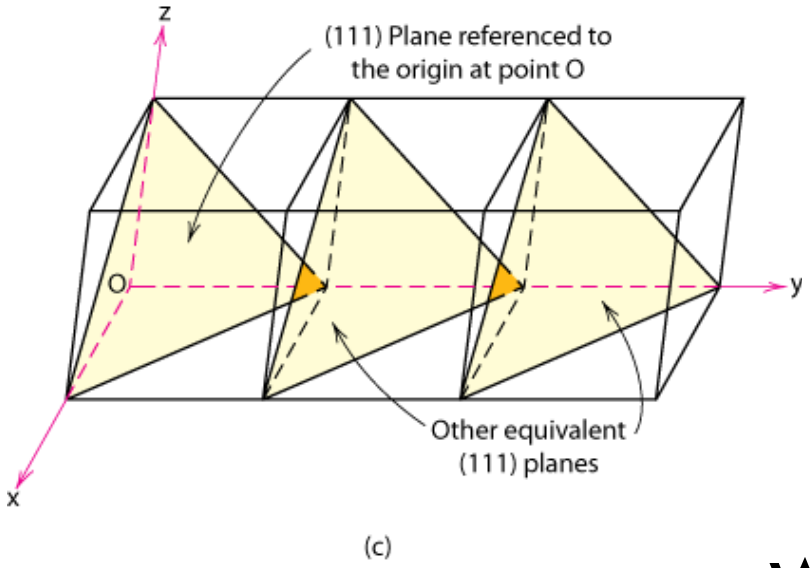
- Determine the indices for this direction
  - Answer: [120]



Crystallographic Planes







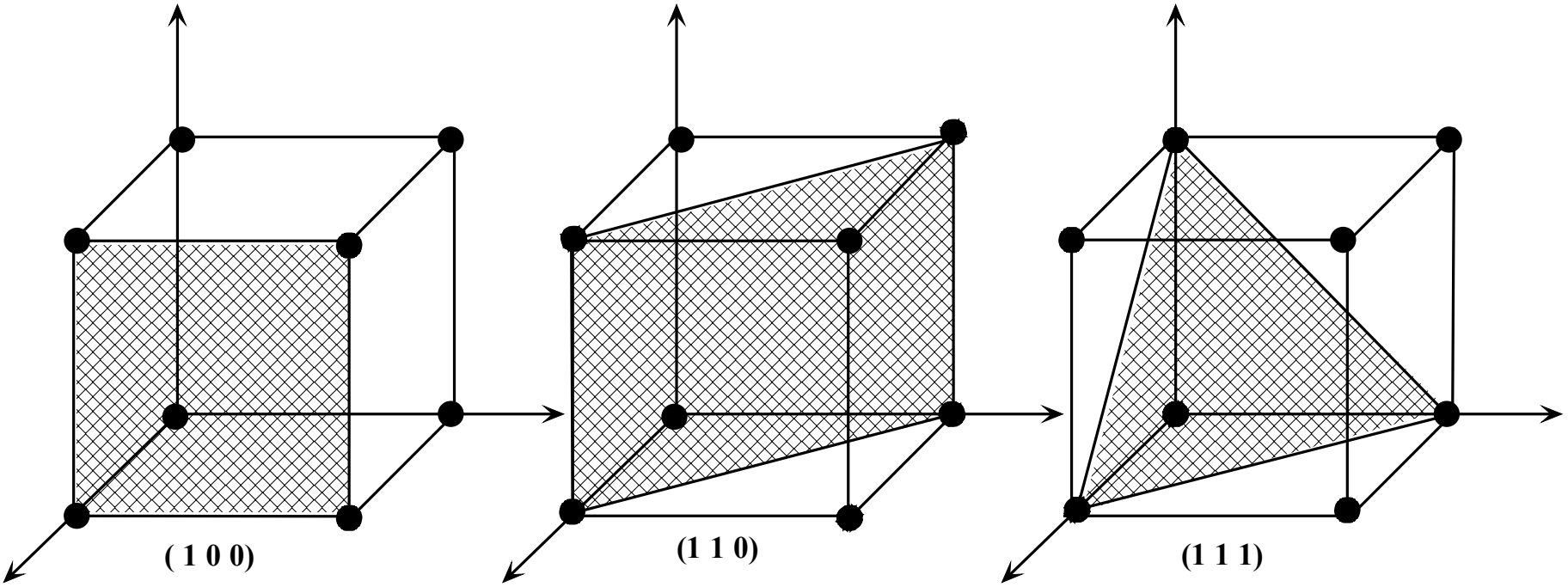
Adapted from Fig. 3.7, *Callister & Rethwisch 9e.*

Crystallographic Planes

- Miller Indices: Reciprocals of the (three) axial intercepts for a plane, cleared of fractions & common multiples. All parallel planes have same Miller indices.

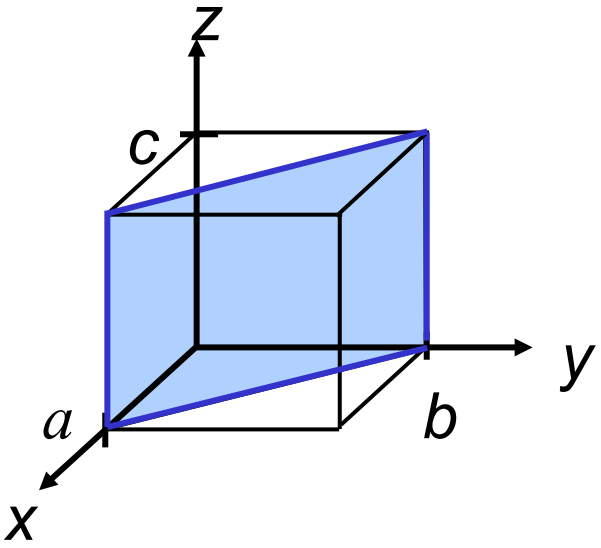
- Algorithm
  1. If plane passes through origin, translate plane or choose new origin
  2. Read off intercepts of plane with axes in terms of a, b, c
  3. **Take reciprocals** of intercepts
  4. Reduce to smallest integer values
  5. Enclose in parentheses, no commas i.e., (*hkl*)

THREE IMPORTANT CRYSTAL PLANES

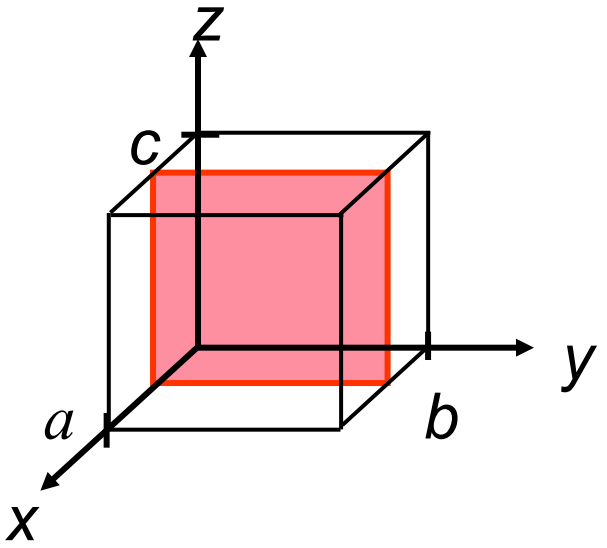


Crystallographic Planes

example		*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)		

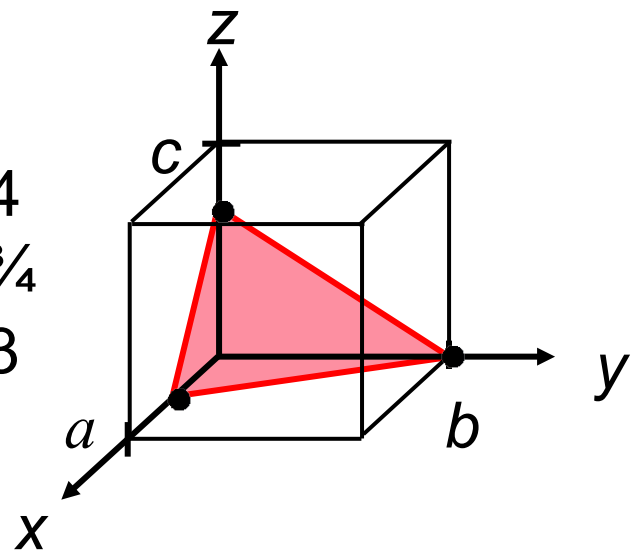


example		*a*	*b*	*c*
1.	Intercepts	1/2	∞	∞
2.	Reciprocals	1/½	1/∞	1/∞
		2	0	0
3.	Reduction	1	0	0
4.	Miller Indices	(100)		



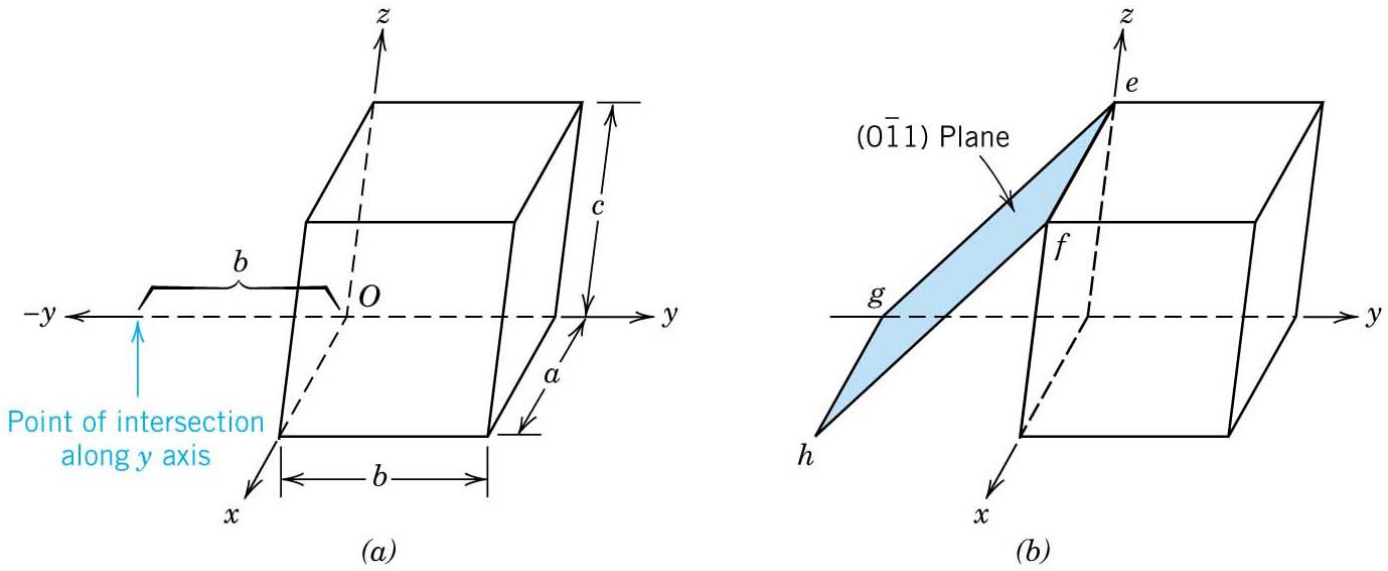
Crystallographic Planes

example	a	b	c
1. Intercepts	1/2	1	3/4
2. Reciprocals	1/½	1/1	1/¾
	2	1	4/3
3. Reduction	6	3	4
4. Miller Indices	(634)		



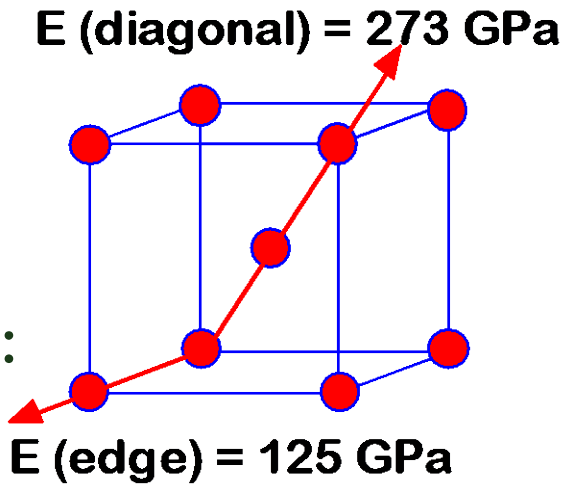
EXAMPLE: CRYSTAL PLANES

- Construct a $(0\bar{1}1)$ plane

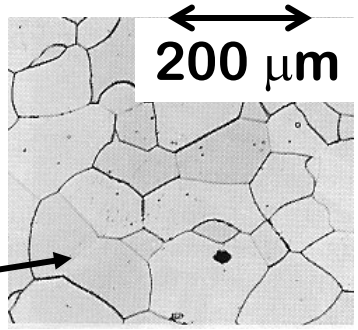


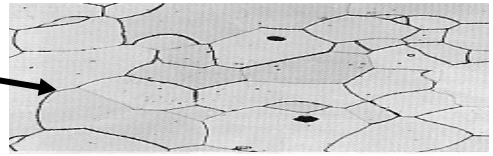
SINGLE VS POLYCRYSTALS

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



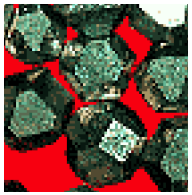
- **Polycrystals**
  - -Properties may/may not vary with direction.
  - -If grains are randomly oriented: isotropic.
    ($E_{poly\ iron}$ = 210 GPa)
  - -If grains are textured, anisotropic.





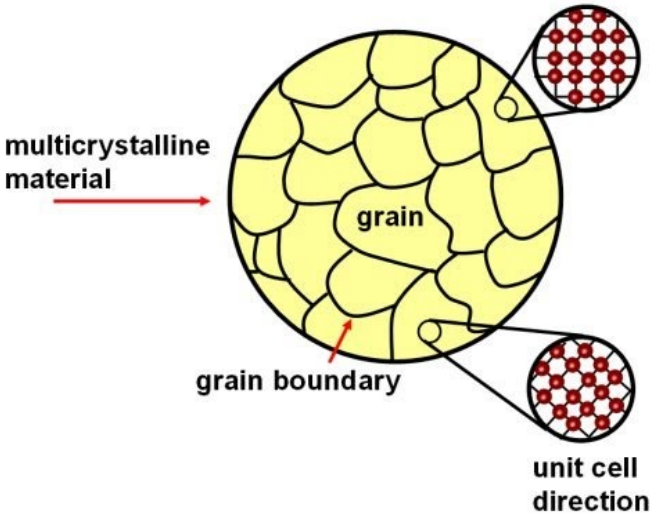
- **Some engineering applications require single crystals:**

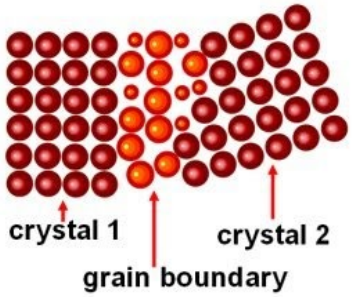
--diamond single crystals for abrasives

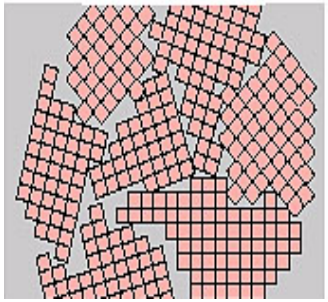


--turbine blades

- **Most engineering materials are polycrystals.**







NOTE (for plane and direction):

- ***PLANE***

  Make sure you enclosed your final answer in brackets / parentheses (…) with no separating commas → (hkl)

- ***DIRECTION***

  Make sure you enclosed your final answer in square brackets […] with no separating commas → [hkl]

- ***FOR BOTH PLANE AND DIRECTION***

  Negative number should be written as follows :

  -1 (WRONG)

  $\bar{1}$ (CORRECT)

Final answer for labeling the plane and direction should not have fraction number → *do a reduction.*

MILLER INDICES OF A **DIRECTION**

How to determine crystal direction indices?

i) Determine the length of the vector projection on each of the three axes, based on $(x_2, y_2, z_2) - (x_1, y_1, z_1)$

ii) These three numbers are expressed as the smallest integers and negative quantities are indicated with an overbar.

iii) Label the direction [hkl].

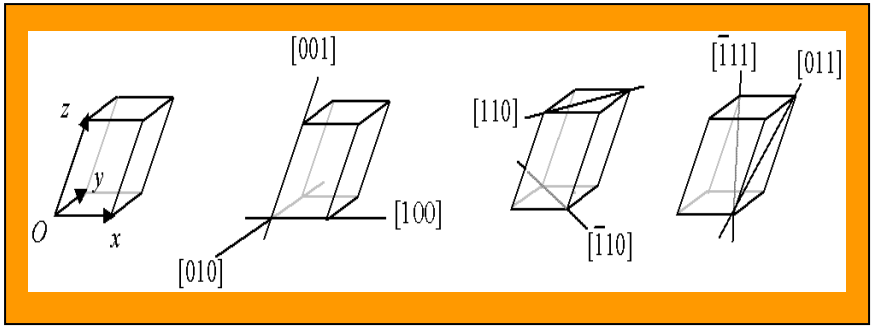


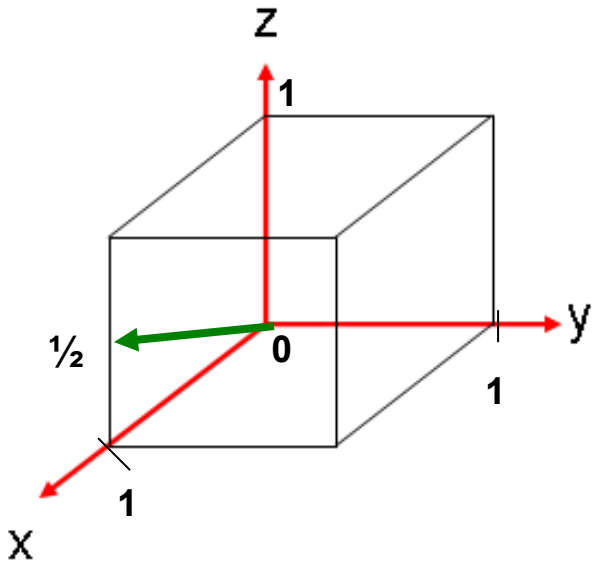
Figure : Examples of direction

Axis	X	Y	Z
Head (H)	x_2	y_2	z_2
Tail (T)	x_1	y_1	z_1
Head (H) –Tail (T)	x_2-x_1	y_2-y_1	z_2-z_1
Reduction *(if necessary)*			
Enclosed	[h	k	l]

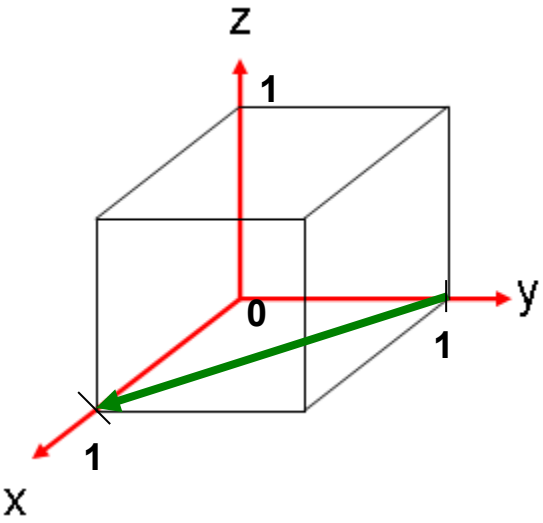
** No reciprocal involved.*

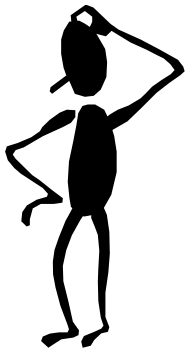
EXAMPLE : CRYSTAL DIRECTION INDICES

Axis	X	Y	Z
Head (H)	1	0	½
Tail (T)	0	0	0
Projection (H-T)	1	0	½
Reduction *(if necessary) * 2*	2	0	1
Enclosed	[2	0	1]



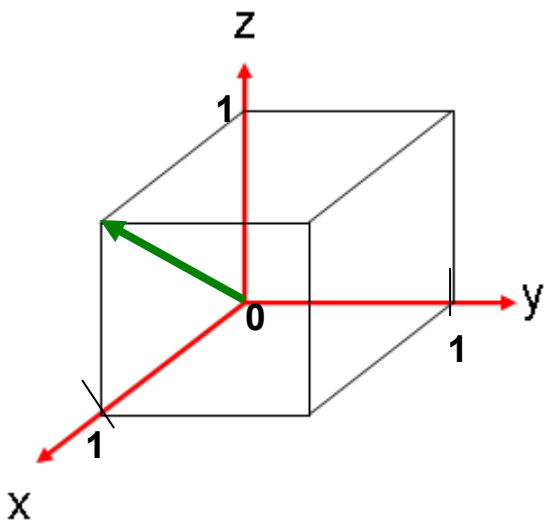
Axis	X	Y	Z
Head (H)	1	0	0
Tail (T)	0	1	0
Projection (H-T)	1	$\bar{1}$	0
Enclosed	[1	$\bar{1}$	0]





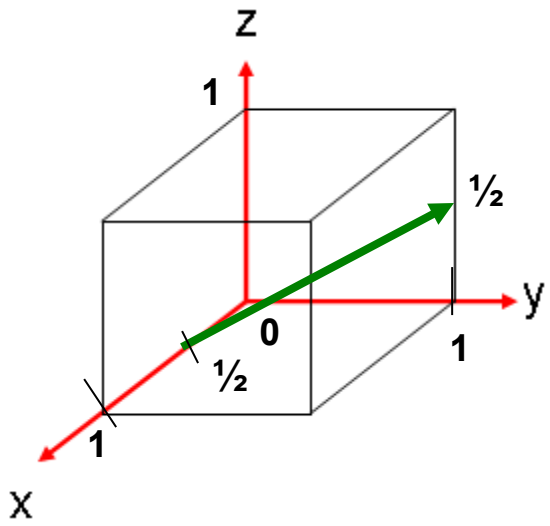
Determine the Miller Indices *direction* for the following figure below?

a)



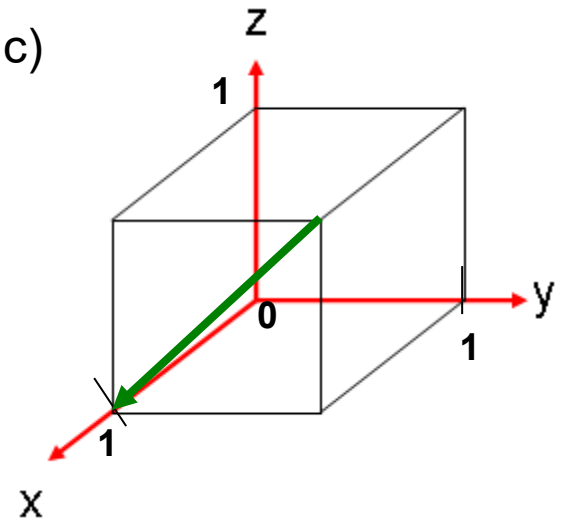
Axis	x	y	z
Head			
Tail			
Projection (Head – Tail)			
Reduction (if necessary)			
Enclosed	[		]

b)



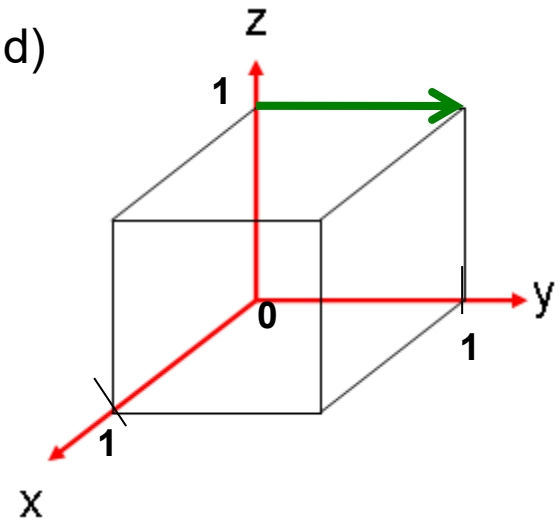
Axis	x	y	z
Head			
Tail			
Projection (Head – Tail)			
Reduction (if necessary)			
Enclosed	[		]

c)



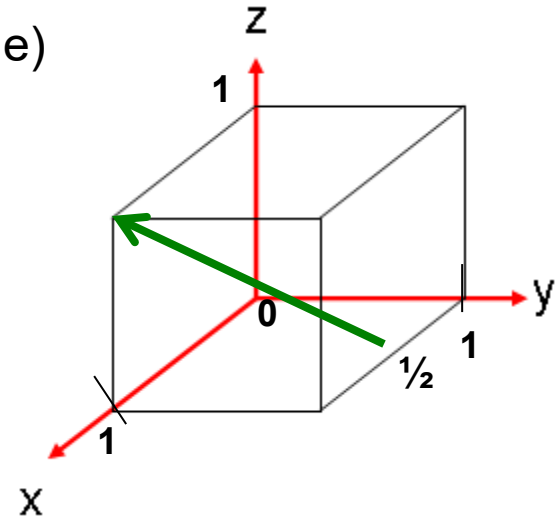
Axis	x	y	z
Head			
Tail			
Projection (Head – Tail)			
Reduction (if necessary)			
Enclosed	[		]

d)

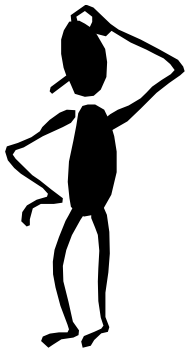


Axis	x	y	z
Head			
Tail			
Projection (Head – Tail)			
Reduction (if necessary)			
Enclosed	[		]

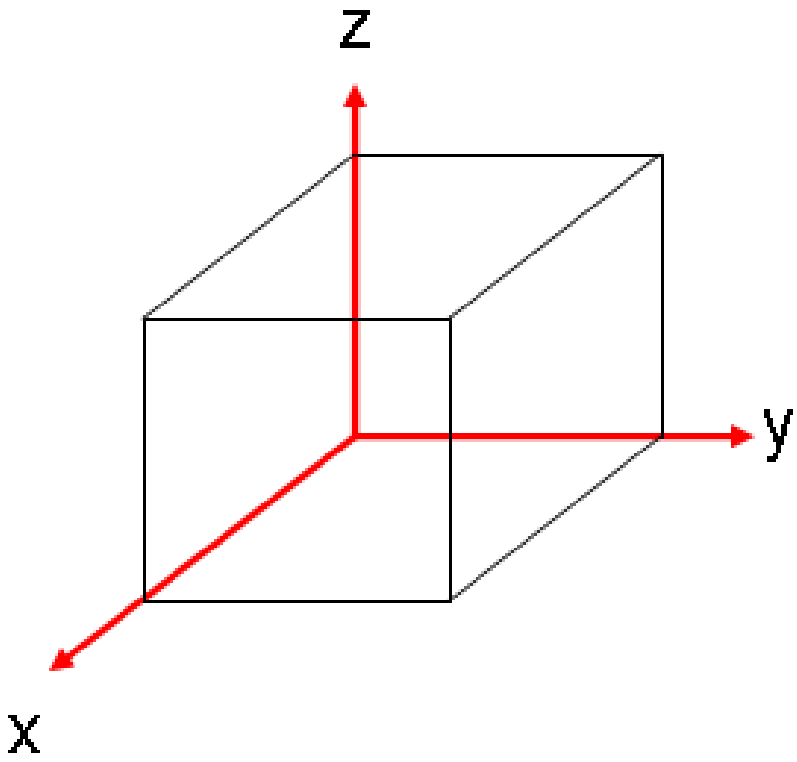
e)



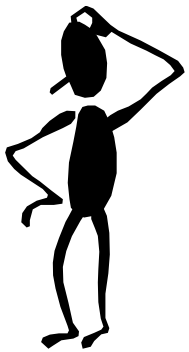
Axis	x	y	z
Head			
Tail			
Projection (Head – Tail)			
Reduction (if necessary)			
Enclosed	[		]



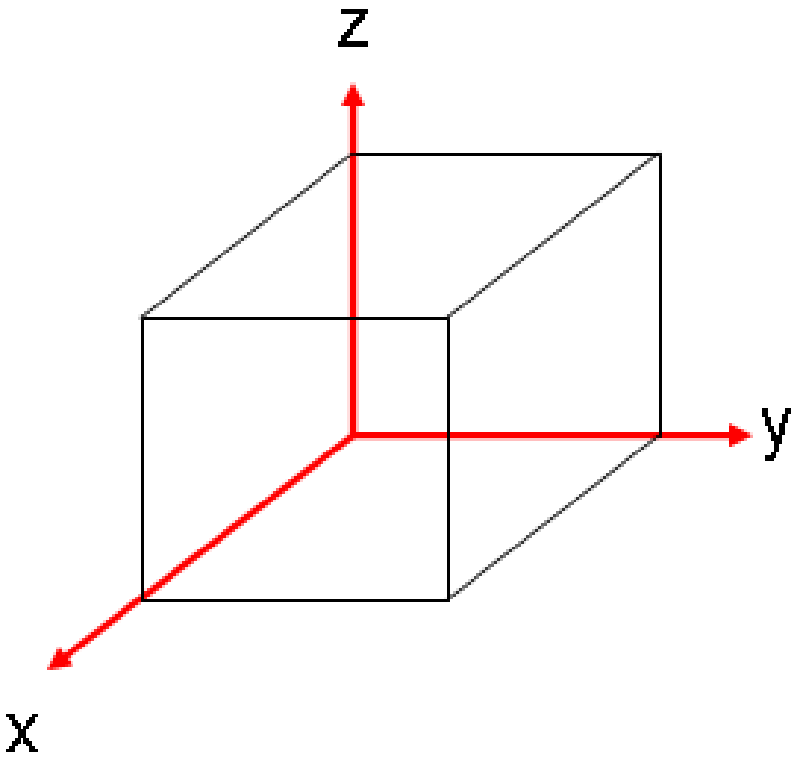
Determine the direction indices of the cubic direction between the position coordinates TAIL (3/4, 0, 1/4) and HEAD (1/4, 1/2, 1/2)? Draw the direction within a unit cell.



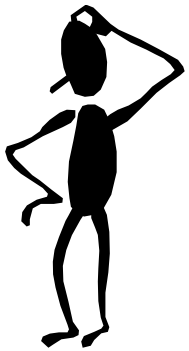
Axis	x	y	z
Head			
Tail			
Projection (Head – Tail)			
Reduction (if necessary)			
Enclosed	[		]



Determine the direction indices of the cubic direction between the position coordinates TAIL (1, 0, 1/2) and HEAD (0, 1, 1/3)? Draw the direction within a unit cell.



Axis	x	y	z
Head			
Tail			
Projection (Head – Tail)			
Reduction (if necessary)			
Enclosed	[		]



Draw the following Miller Indices *direction.*

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

b)[1 1 1]

c)[1 1 2]

MILLER INDICES OF A **PLANE**

How to determine crystal plane indices?

i) Determine the points at which a given crystal plane intersects the three axes, say at (a,0,0),(0,b,0), and (0,0,c). If the plane is parallel an axis, it is given an intersection ∞.

ii) Take the reciprocals of the three integers found in step (i).

iii) Label the plane (hkl). These three numbers are expressed as the smallest integers and negative quantities are indicated with an overbar,e.g : $\overline{a}$.

Axis	**X**	**Y**	**Z**
Interceptions			
Reciprocals			
Reduction ***(if necessary)***			
Enclosed	**(h**	**k**	**l)**

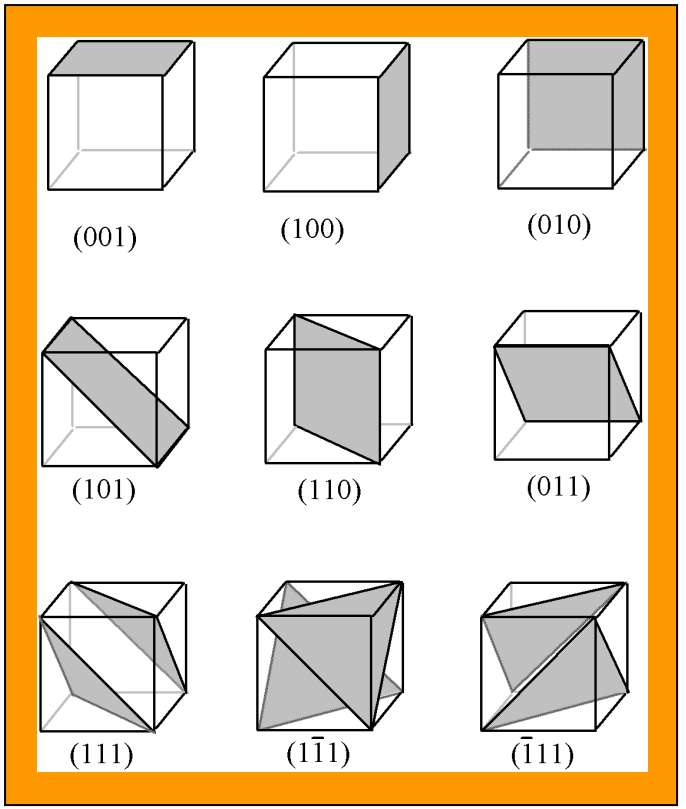
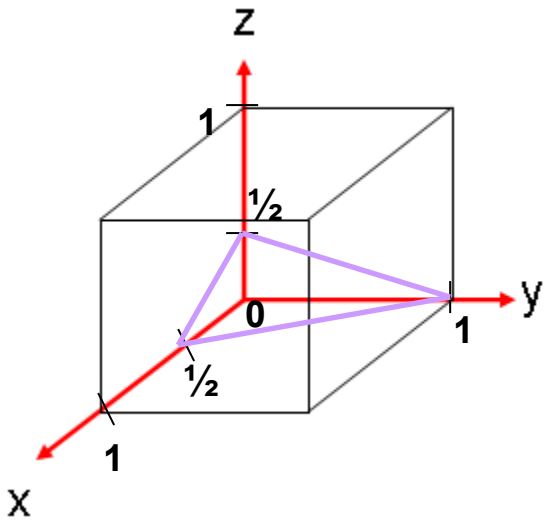


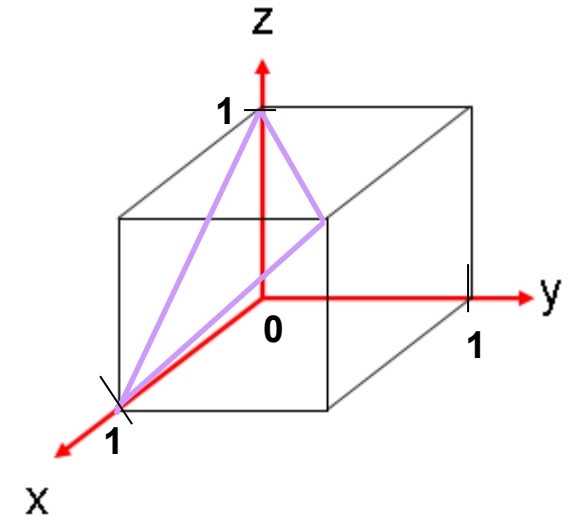
Figure : Planes with different Miller indices in cubic crystals

EXAMPLE : CRYSTAL PLANE INDICES

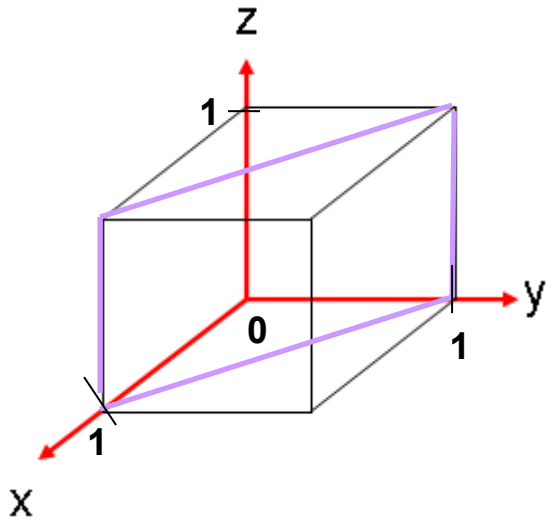
Axis	X	Y	Z
Interceptions	½	1	½
Reciprocals	2	1	2
Reduction *(if necessary)*			
Enclosed	(2	1	2)



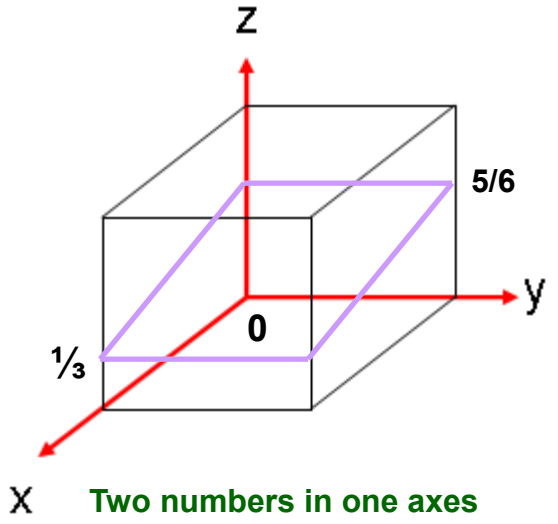
Axis	X	Y	Z
Interceptions	$\overline{1}$	1	$\overline{1}$
Reciprocals			
Reduction *(if necessary)*			
Enclosed	($\overline{1}$	1	$\overline{1}$)



Axis	X	Y	Z
Interceptions	1	1	∞
Reciprocals	1	1	0
Reduction *(if necessary)*			
Enclosed	(1	1	0)

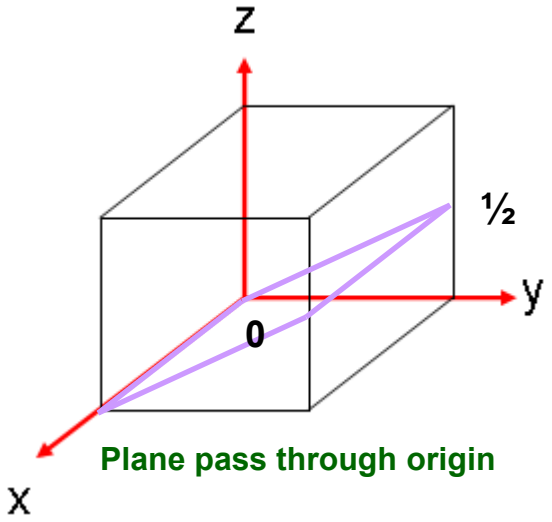


Axis	X	Y	Z
Interceptions	1	∞	½
Reciprocals	1	0	2
Reduction *(if necessary)*			
Enclosed	(1	0	2)



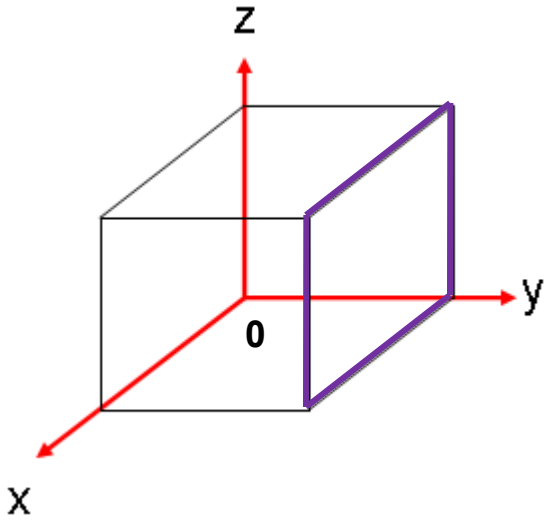
Two numbers in one axes

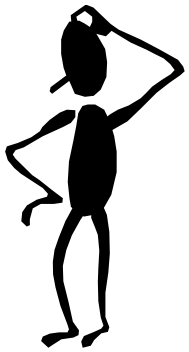
Axis	X	Y	Z
Interceptions	∞	1	½
Reciprocals	0	1	2
Reduction *(if necessary)*			
Enclosed	(0	1	2)



Plane pass through origin

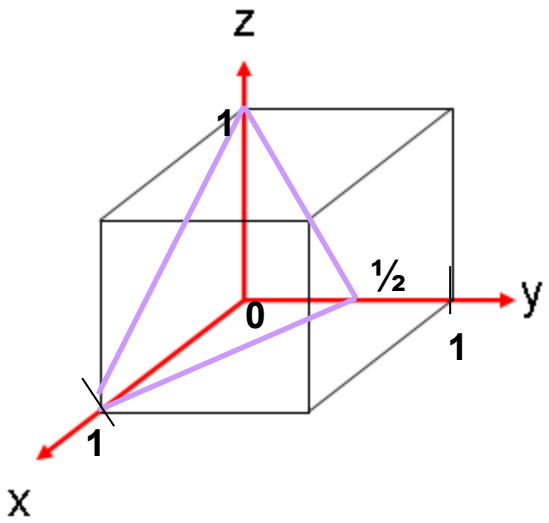
Axis	X	Y	Z
Interceptions	∞	1	∞
Reciprocals	0	1	0
Reduction *(if necessary)*			
Enclosed	(0	1	0)





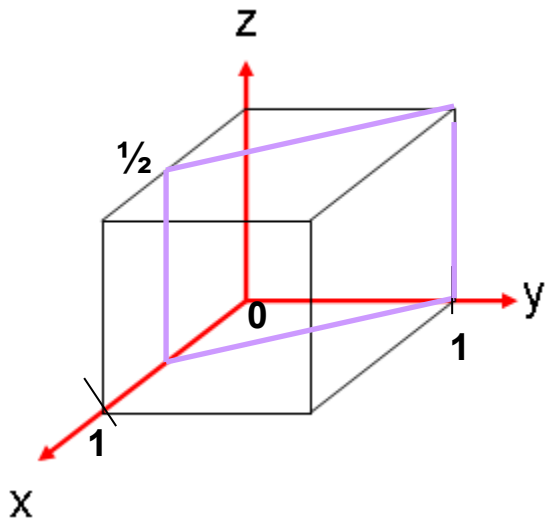
Determine the Miller Indices *plane* for the following figure below?

a)



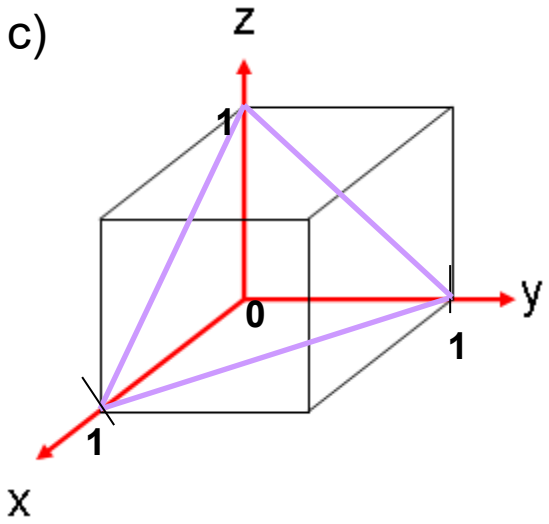
Axis	x	y	z
Intercepts			
Reciprocals			
Reduction (if necessary)			
Enclosed	(		)

b)



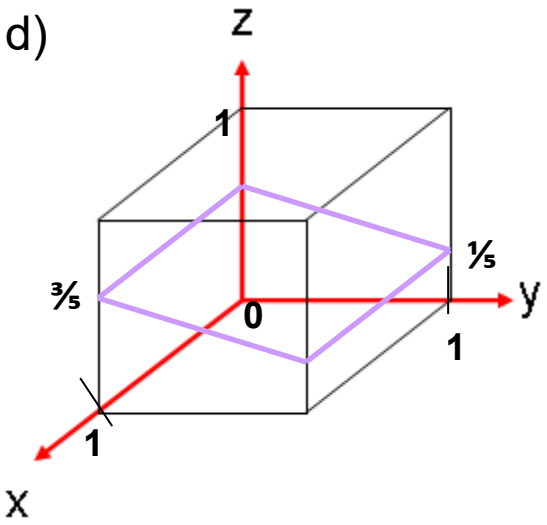
Axis	x	y	z
Intercepts			
Reciprocals			
Reduction (if necessary)			
Enclosed	(		)

c)

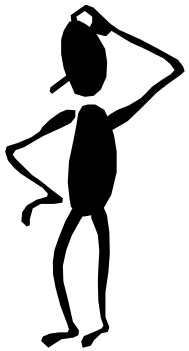


Axis	x	y	z
Intercepts			
Reciprocals			
Reduction (if necessary)			
Enclosed	(		)

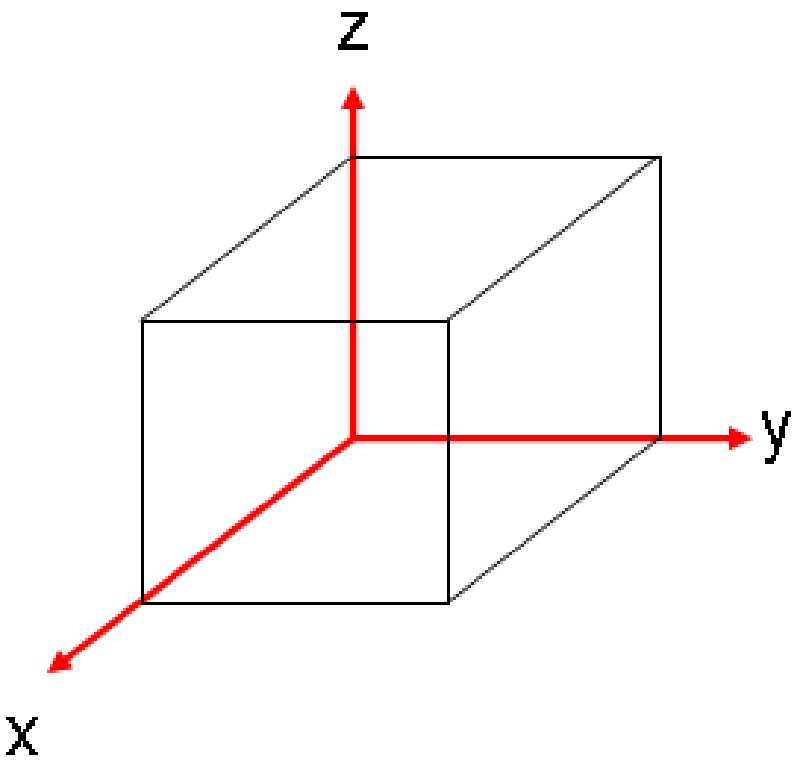
d)



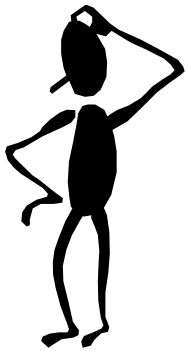
Axis	x	y	z
Intercepts			
Reciprocals			
Reduction (if necessary)			
Enclosed	( )		



Determine the Miller indices of a cubic crystal plane that intersects the position coordinates A (1, 1/4, 0), B (1, 1, 1/2) , C (3/4, 1, 1/4) and D (1/2, 1, 0) ? Draw the plane.



Axis	x	y	z
Intercepts			
Reciprocals			
Reduction (if necessary)			
Enclosed	(		)



Draw the following Miller Indices *plane.*

a) (1 0 1)

b) (1 $\bar{1}$ 0)

c) (0 $\bar{1}$ 1)

d) (2 2 1)

e) (1 3 1)

Summary

- Atoms may assemble into crystalline or amorphous structures.
- Crystallographic points, directions and planes are specified in terms of indexing schemes. Crystallographic directions and planes are related to atomic linear densities and planar densities.
- Materials can be single crystals or polycrystalline. Material properties generally vary with single crystal orientation (i.e., they are anisotropic), but are generally non-directional (i.e., they are isotropic) in polycrystals with randomly oriented grains.