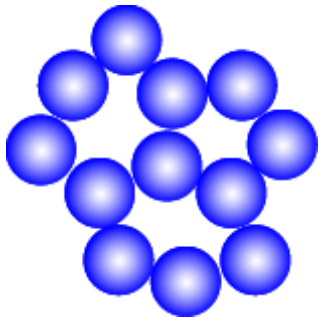
Chapter 3: Fundamentals of Crystallography

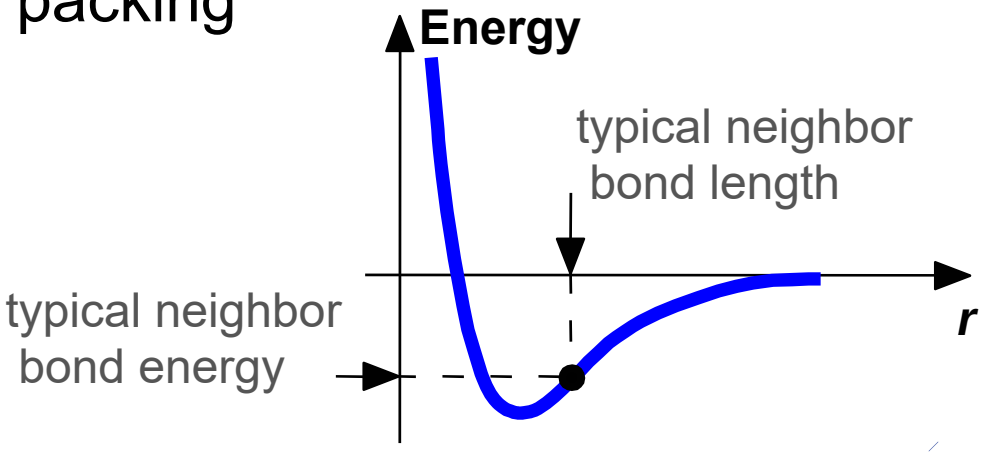
ISSUES TO ADDRESS...

- 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?

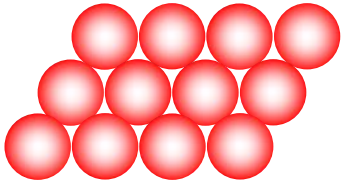
Energy and Packing

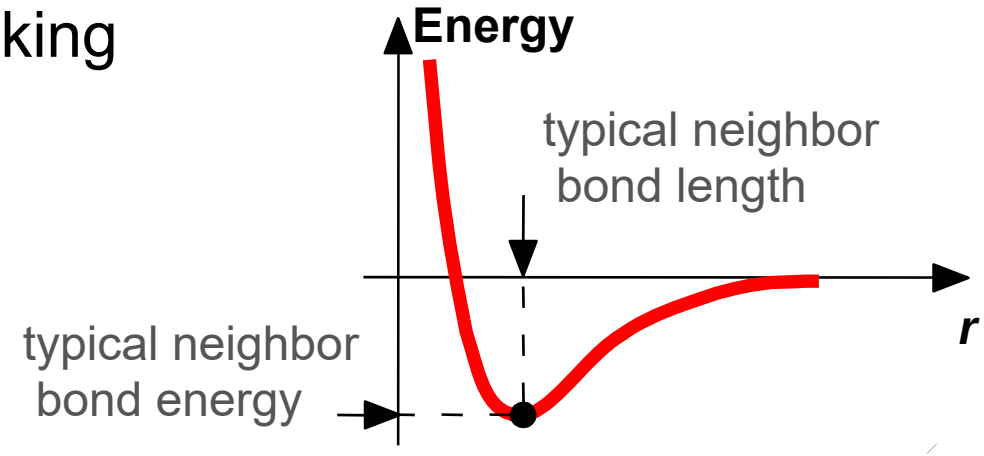
- Non dense, random packing





- Dense, ordered packing



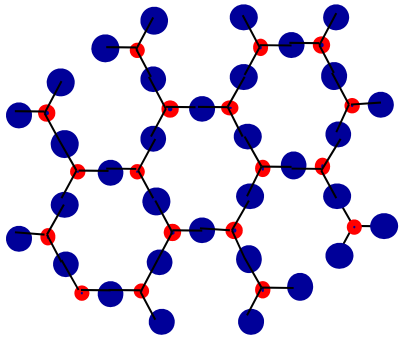


Dense, ordered packed structures tend to have lower energies.

Materials and Packing

Crystalline materials...

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



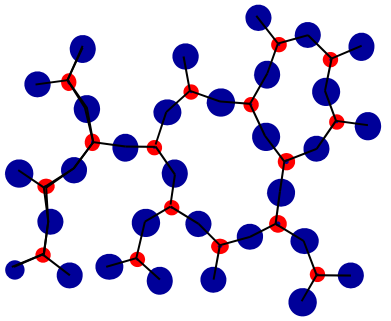
crystalline SiO_2

Adapted from Fig. 3.23(a), *Callister & Rethwisch 8e.*

• Si • Oxygen

Noncrystalline materials...

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



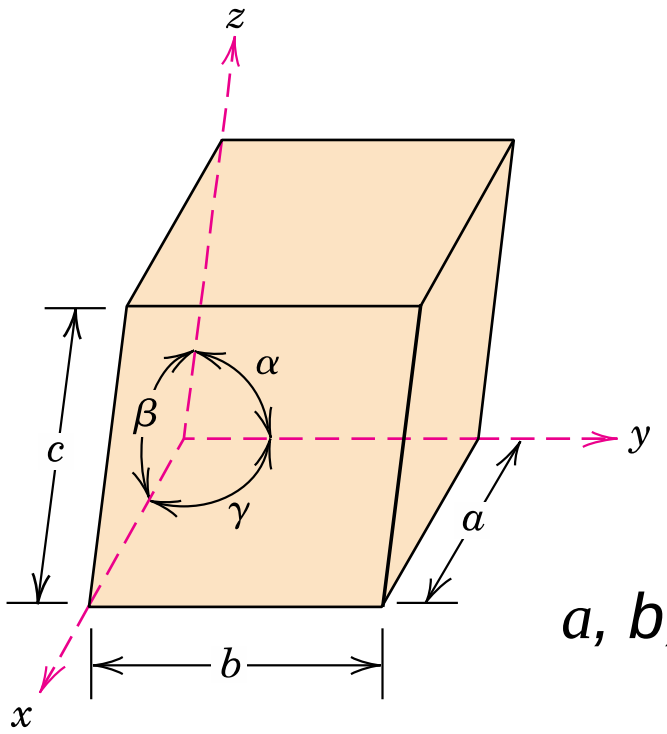
noncrystalline SiO_2

Adapted from Fig. 3.23(b), *Callister & Rethwisch 8e.*

"Amorphous" = Noncrystalline
= Vitreous = Glassy

Crystal Systems

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

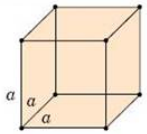
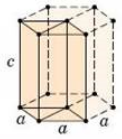
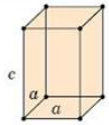
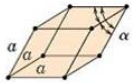
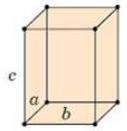
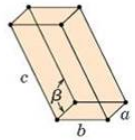
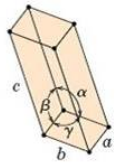


7 crystal systems

14 crystal lattices

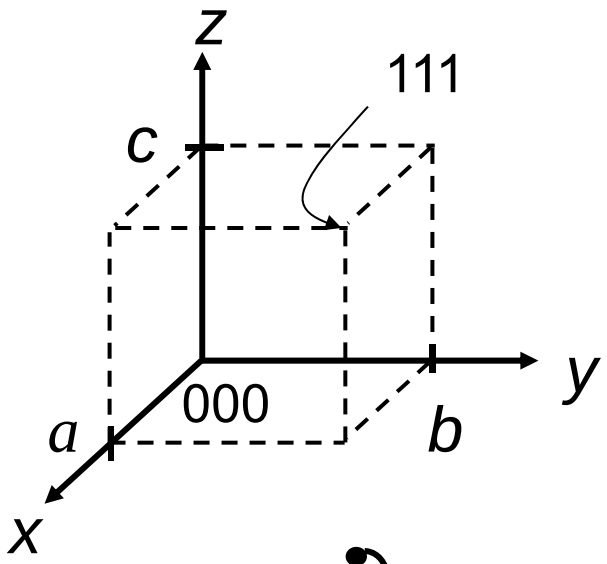
a, *b*, and *c* are the lattice constants

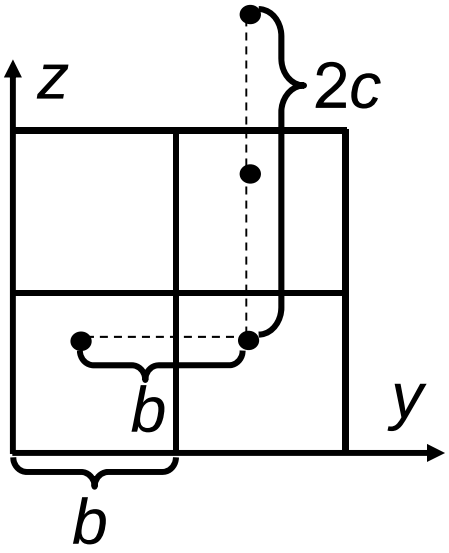
Table 3.1 Lattice Parameter Relationships and Figures Showing Unit Cell Geometries for the Seven Crystal Systems

Crystal System	*Axial Relationships*	*Interaxial Angles*	*Unit Cell Geometry*
Cubic	$a = b = c$	$\alpha = \beta = \gamma = 90°$	
Hexagonal	$a = b \neq c$	$\alpha = \beta = 90°, \gamma = 120°$	
Tetragonal	$a = b \neq c$	$\alpha = \beta = \gamma = 90°$	
Rhombohedral (Trigonal)	$a = b = c$	$\alpha = \beta = \gamma \neq 90°$	
Orthorhombic	$a \neq b \neq c$	$\alpha = \beta = \gamma = 90°$	
Monoclinic	$a \neq b \neq c$	$\alpha = \gamma = 90° \neq \beta$	
Triclinic	$a \neq b \neq c$	$\alpha \neq \beta \neq \gamma \neq 90°$	

WileyPLUS: VMSE
Crystal Systems and Unit Cells for Metals

Point Coordinates





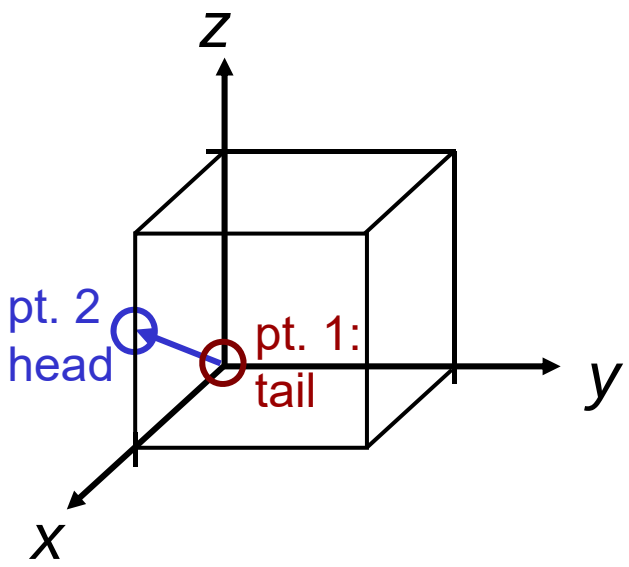
Point coordinates for unit cell center are

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

Crystallographic Directions



ex:

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

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

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

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:

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

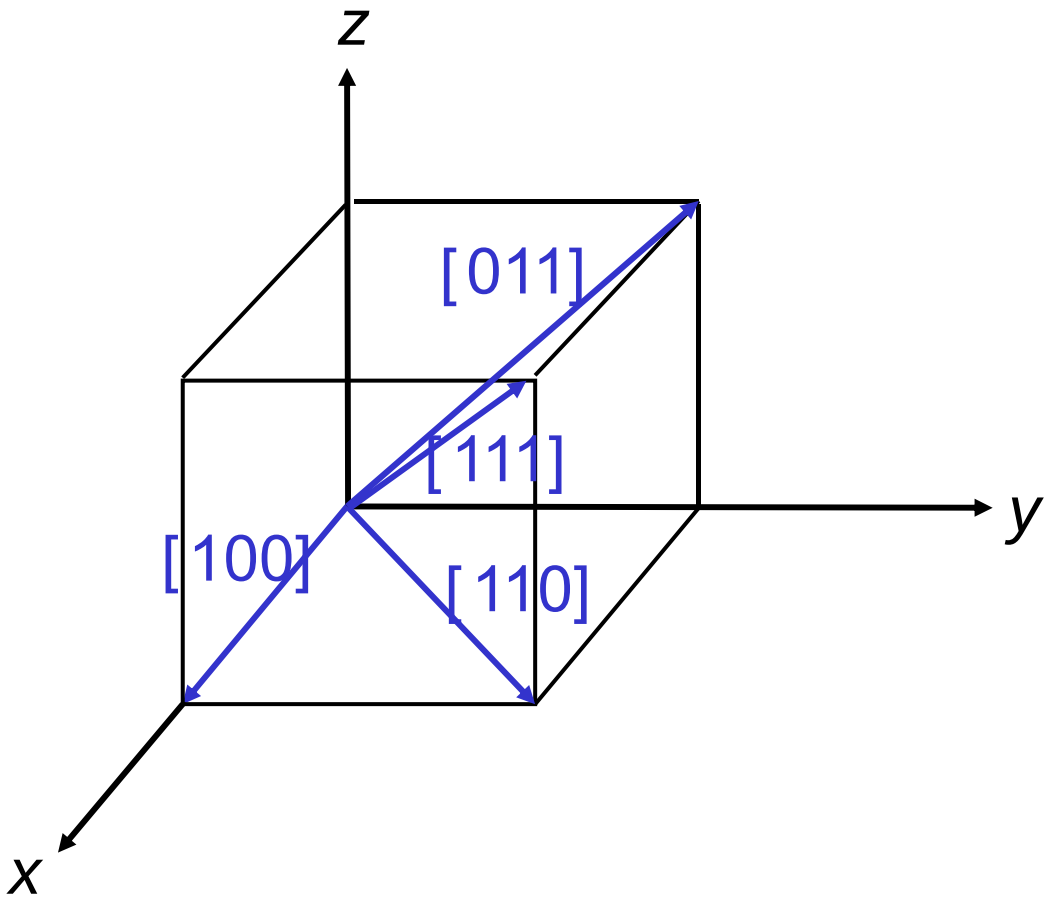
4. Adjust to smallest integer values
5. Enclose in square brackets, no commas

[*uvw*]

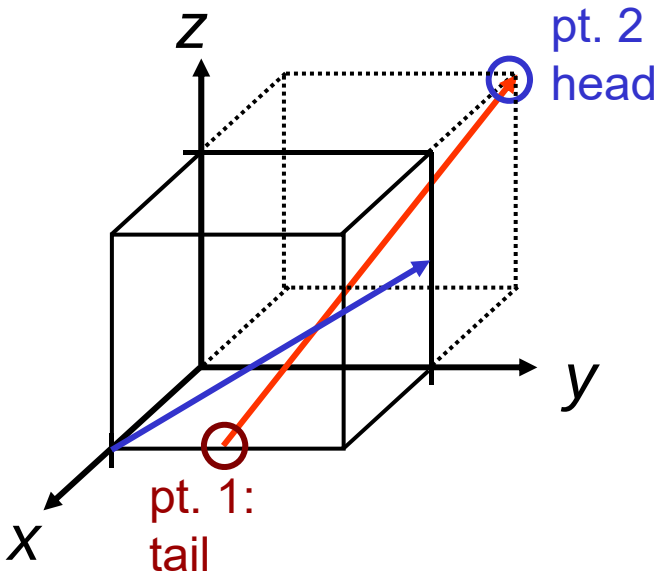
=> 1, 0, 1/2 => 2, 0, 1

=> [201]

Crystallographic Directions



Crystallographic Directions



Example 2:

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

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

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

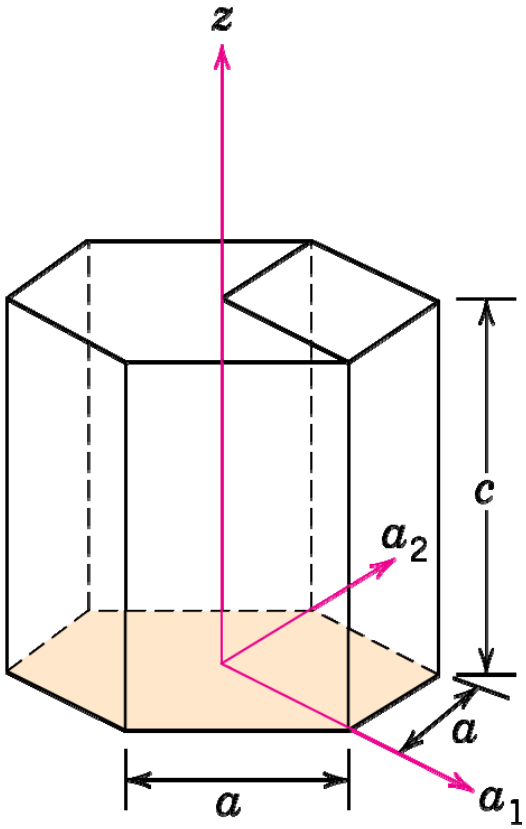
=> -2, 1/2, 1

Multiplying by 2 to eliminate the fraction

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

families of directions <*uvw*>

Determination of HCP Crystallographic Directions



Algorithm

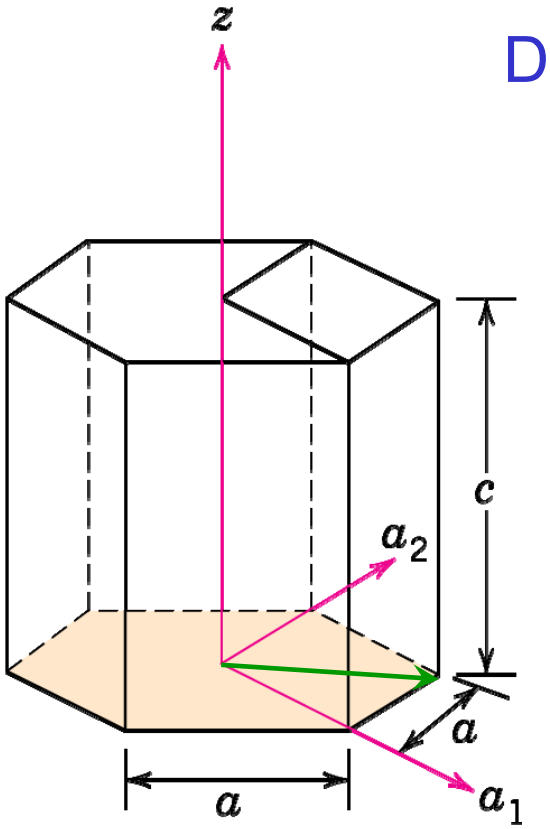
1. Determine coordinates of vector tail, pt. 1: x_1, y_1, & z_1; and vector head, pt. 2: x_2, y_2, & z_2. in terms of three axis (a_1, a_2, and z)
2. Tail point coordinates subtracted from head point coordinates and normalized by unit cell dimensions a and c
3. Adjust to smallest integer values
4. Enclose in square brackets, no commas, for three-axis coordinates $[u'v'w']$
5. Convert to four-axis Miller-Bravais lattice coordinates using equations below:

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

$$t = -(u + v) \qquad w = w'$$

6. Adjust to smallest integer values and enclose in brackets [*uvtw*]

Determination of HCP Crystallographic Directions



Determine indices for green vector

Example		a_1	a_2	z
1.	Tail location	0	0	0
	Head location	a	a	$0c$
2.	Normalized	1	1	0
3.	Reduction	1	1	0
4.	Brackets		[110]	

5. Convert to 4-axis parameters

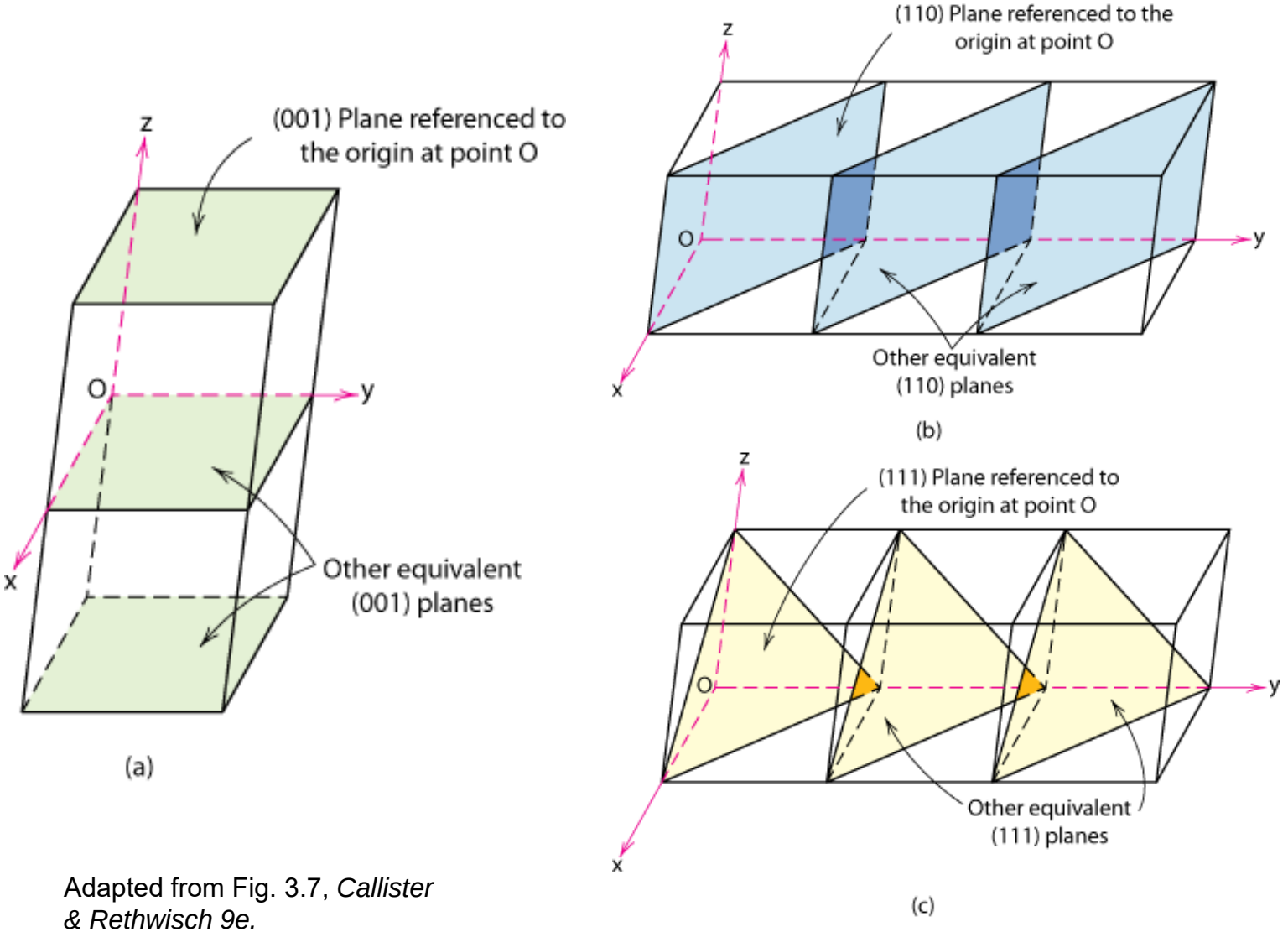
$$u = \frac{1}{3}[(2)(1)-(1)] = \frac{1}{3} \qquad v = \frac{1}{3}[(2)(1)-(1)] = \frac{1}{3}$$

$$t = -(\frac{1}{3}+\frac{1}{3}) = -\frac{2}{3} \qquad w = 0$$

6. Reduction & Brackets

1/3, 1/3, -2/3, 0 => 1, 1, -2, 0 => $[11\bar{2}0]$

Crystallographic Planes



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

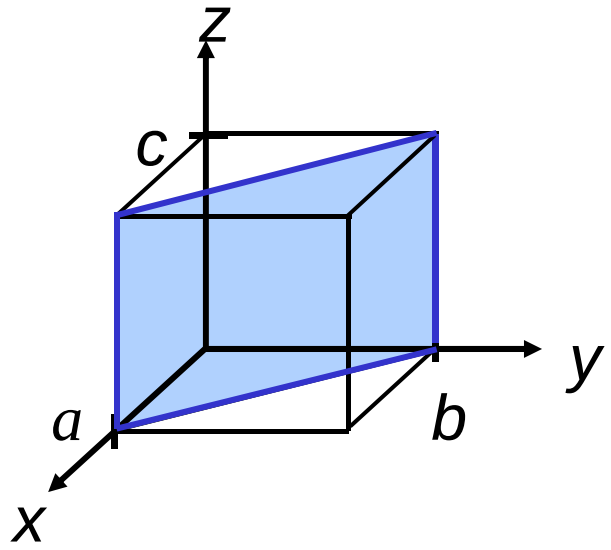
Crystallographic Planes

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

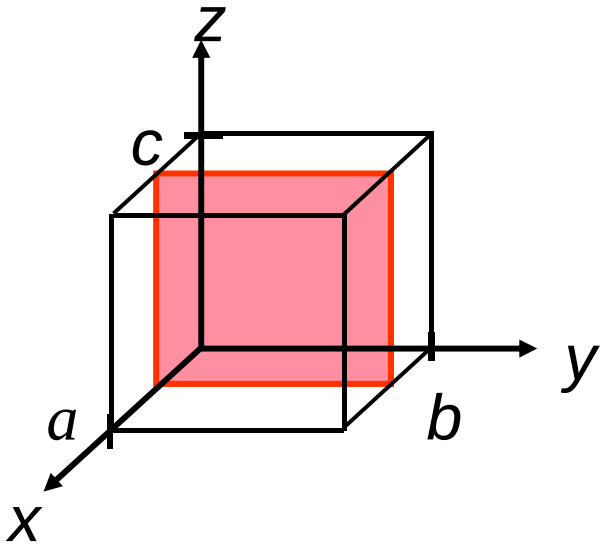
- Algorithm
  1. Read off intercepts of plane with axes in terms of a, b, c
  2. Take reciprocals of intercepts
  3. Reduce to smallest integer values
  4. Enclose in parentheses, no commas i.e., (*hkl*)

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)		

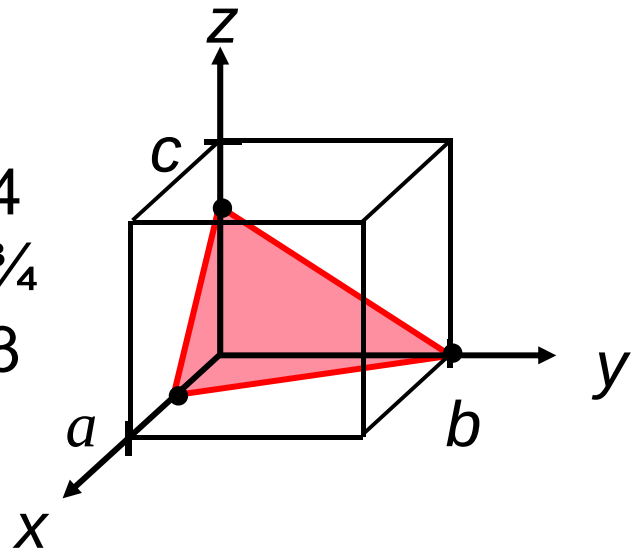


example		*a*	*b*	*c*
1.	Intercepts	1/2	∞	∞
2.	Reciprocals	1/½	1/∞	1/∞
		2	0	0
3.	Reduction	2	0	0
4.	Miller Indices	(100)		



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)		



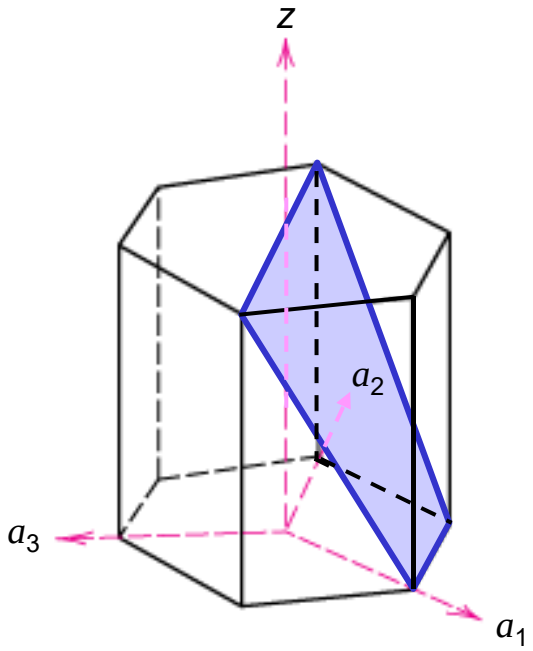
Family of Planes {*hkl*}

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

Crystallographic Planes (HCP)

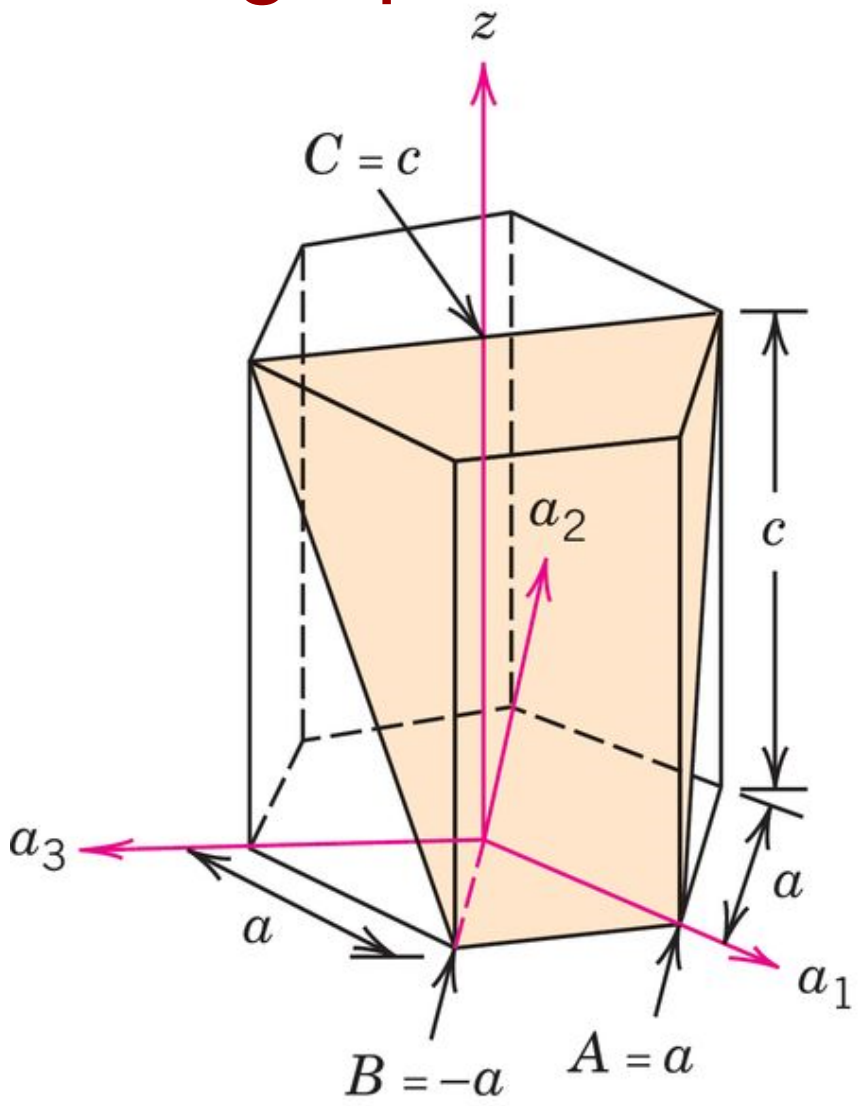
- In hexagonal unit cells the same idea is used

example		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,
Callister & Rethwisch 9e.

Crystallographic Planes (HCP)



Single Crystalline vs. Polycrystalline

Photograph courtesy of Irocks.com, Megan Foreman photo.

Fig_03_09

(d)

Courtesy of Irocks.com

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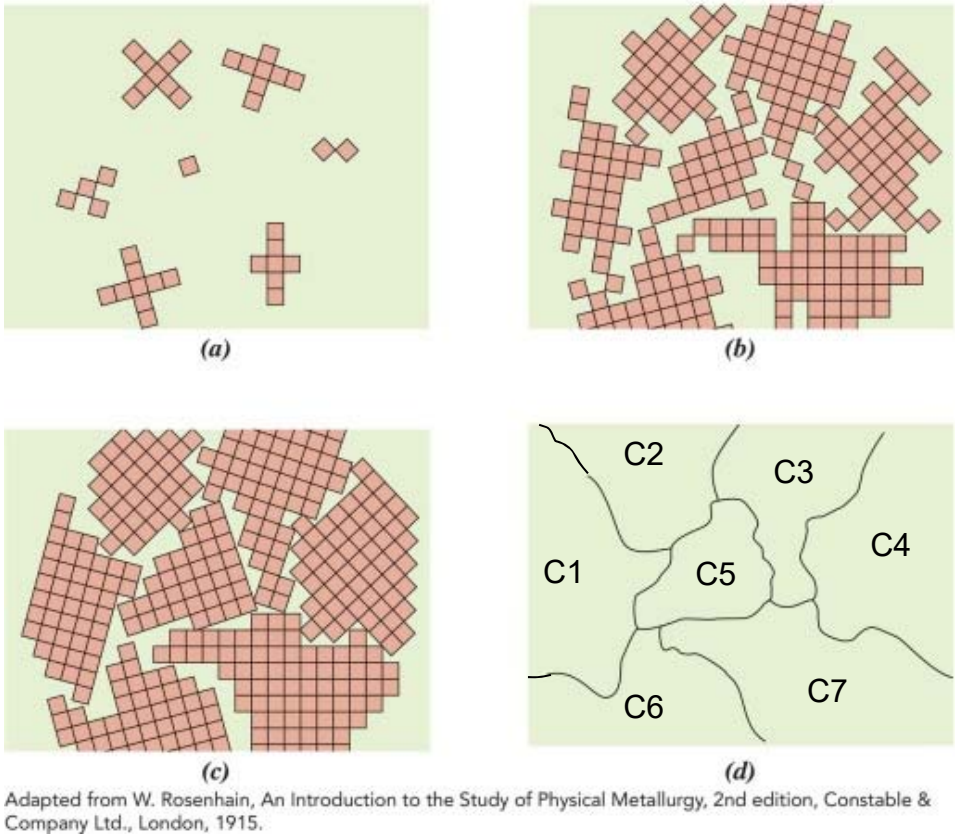
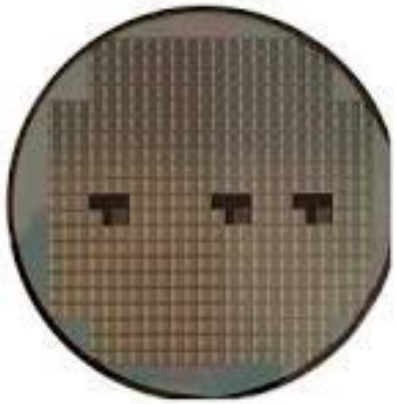
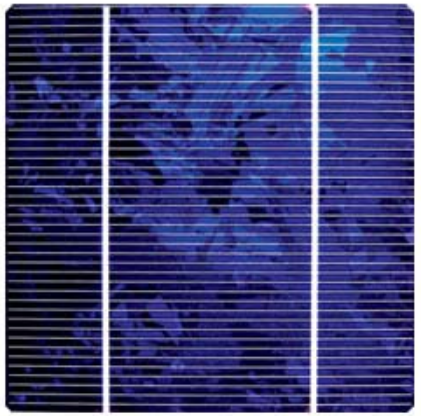


Adapted from W. Rosenhain, An Introduction to the Study of Physical Metallurgy, 2nd edition, Constable & Company Ltd., London, 1915.

Fig_03_10

Single Crystalline vs. Polycrystalline





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.