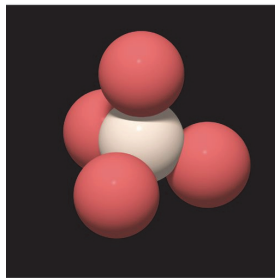


Chapter 3: Fundamentals of Crystallography

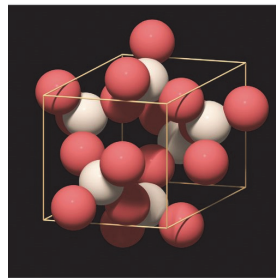
❑ ISSUES TO ADDRESS...

- ❖ 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?



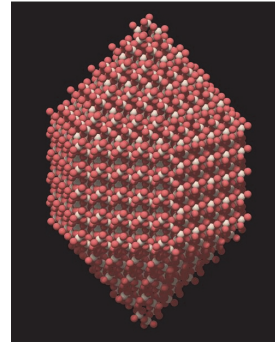
(a)

Courtesy of Amir C. Akhavan



(b)

Courtesy of Amir C. Akhavan



(c)

Courtesy of Amir C. Akhavan



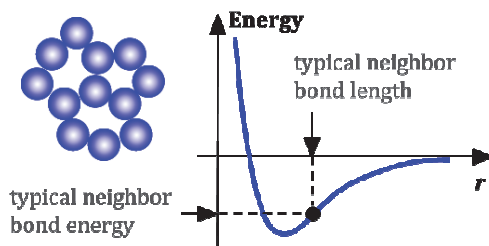
(d)

Courtesy of iStocks.com

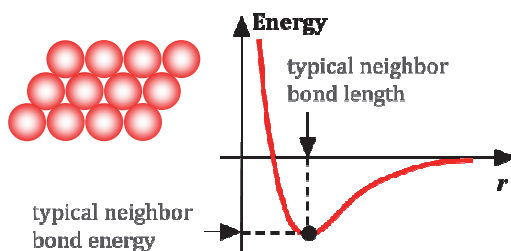
The structure of quartz (SiO_2) from three different dimensional perspectives

Energy, Materials, and Packing

❑ Non-dense, random packing



❑ Dense, ordered packing



❑ Dense, ordered packed structures tend to have lower energies.

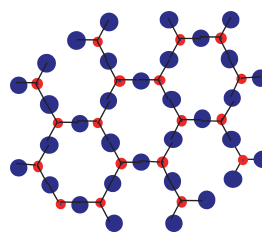
❑ Crystalline materials

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

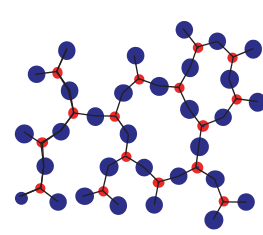
❑ Noncrystalline materials

- ❖ atoms have no periodic packing
- ❖ occurs for complex structures and rapidly cooled materials

❑ "Amorphous" = Noncrystalline



crystalline SiO_2



noncrystalline SiO_2

● Si
● Oxygen

Fundamentals Concepts and Unit Cells

3.2 Fundamental Concepts

- ❖ **Crystalline materials:** The atoms are situated in a repeating or periodic array over large atomic distances.
- ❖ **Noncrystalline or amorphous materials:** The long-range atomic order is absent.

3.3 Unit Cells

- ❖ The smallest repetitive volume which contains the complete lattice pattern of a crystal.
- ❖ The basic structural unit or building block of crystal structures.

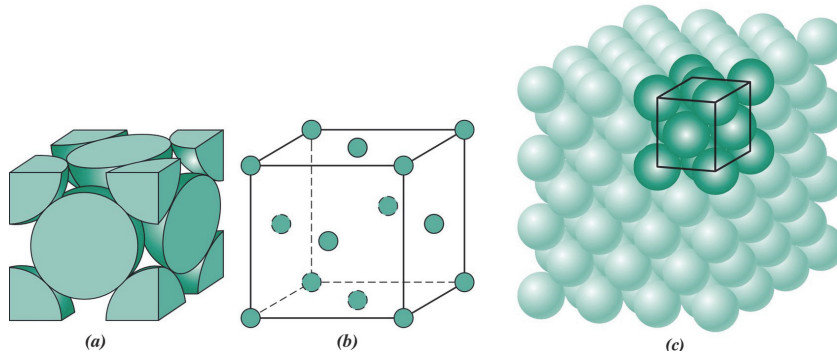


Fig. 3.1 For the face-centered cubic crystal structure, (a) a hard-sphere unit cell representation, (b) a reduced-sphere unit cell, and (c) an aggregate of many atoms.

3.4 Crystal Systems

□ The unit cell geometry is completely defined in terms of the lattice parameters

- ❖ Three edge lengths: a , b , c
- ❖ Three interaxial angles: α , β , γ

Copyright © The McGraw-Hill Companies, Inc. Permission required for reproduction or display.

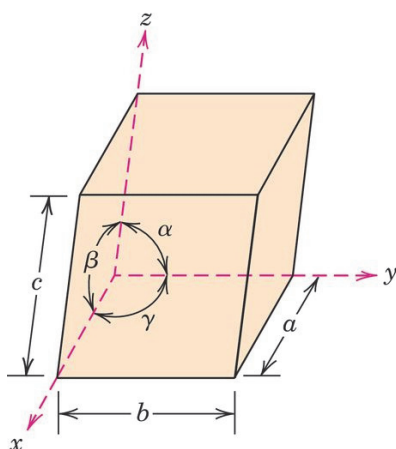
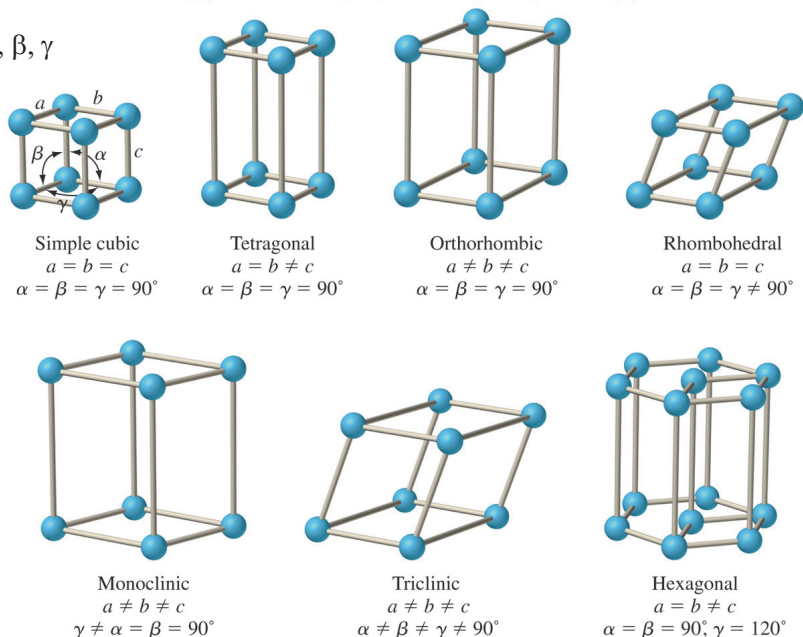


Fig. 3.2 A unit cell with x , y , and z coordinate axes, showing axial lengths (a , b , and c) and interaxial angles (α , β , and γ).



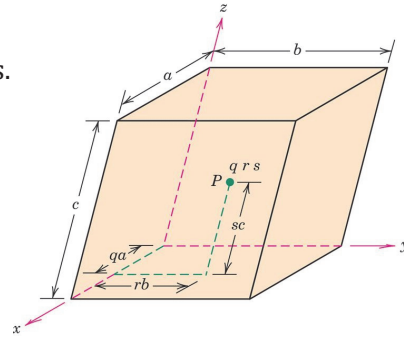
Seven crystal systems

<https://www.wiley.com/college/callister/0470125373/vmse/>

3.5 Point Coordinates

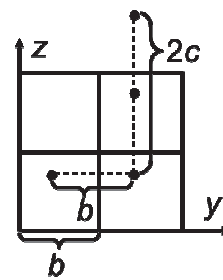
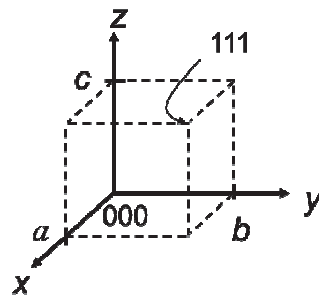
❑ Three point coordinate indices: q, r, and s

- ❖ Fractional multiples of a, b, and c unit cell edge lengths.
- ❖ qa = lattice position referenced to the x axis
- ❖ rb = lattice position referenced to the y axis
- ❖ sc = lattice position referenced to the z axis



❑ Ex. 3.1 & Ex. 3.2

- ❑ Point coordinates for unit cell center are $a/2, b/2, c/2$: $\frac{1}{2} \frac{1}{2} \frac{1}{2}$
- ❑ Point coordinates for unit cell corner are 111.
- ❑ Translation: integer multiple of lattice constants $\rightarrow$ identical position in another unit cell.



3.6 Crystallographic Directions

❑ A crystallographic direction: A line directed between two points or a vector.

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.

$$u = n \left(\frac{x_2 - x_1}{a} \right), \quad v = n \left(\frac{y_2 - y_1}{b} \right), \quad w = n \left(\frac{z_2 - z_1}{c} \right)$$

5. Enclose in square brackets, no commas: $[uvw]$

❑ Family of Crystallographic Directions: $\langle uvw \rangle$

- ❖ Ex: $\langle 100 \rangle = [100], [010], [001], [\bar{1}00], [0\bar{1}0], [00\bar{1}]$

❑ Practice with Examples 3.3 & 3.4.

3.6 Crystallographic Directions (HCP)

❑ Miller-Bravais coordinate system (four axes)

- ❖ The three a_1 , a_2 , and a_3 are all contained within the basal plane.
- ❖ The z axis is perpendicular to this basal plane.
- ❖ Conversion from the three-index system to the four-index system.

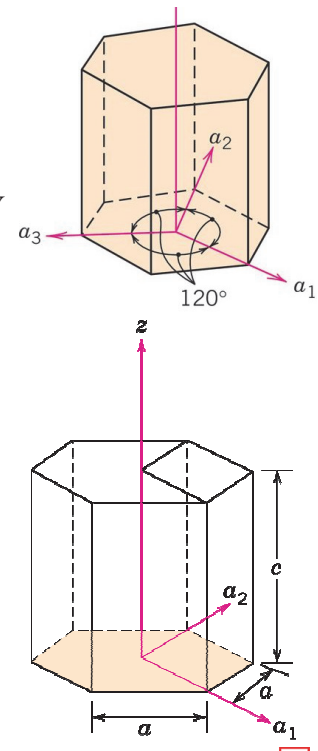
$$[UVW] \rightarrow [uvtw]: \quad u = \frac{1}{3}(2U - V), \quad v = \frac{1}{3}(2U - V), \quad t = -(u + v), \quad w = W$$

❑ 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. $[UVW]$
5. Convert to four-axis Miller-Bravais lattice coordinates using equations below:

$$u = \frac{1}{3}(2U - V), \quad v = \frac{1}{3}(2U - V), \quad t = -(u + v), \quad w = W$$

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



3.7 Crystallographic Planes

❑ Miller Indices

- ❖ Reciprocals of the (three) axial intercepts for a plane, cleared of fractions & common multiples. All parallel planes have the 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)

❑ Family of Crystallographic Planes: $\{hkl\}$

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

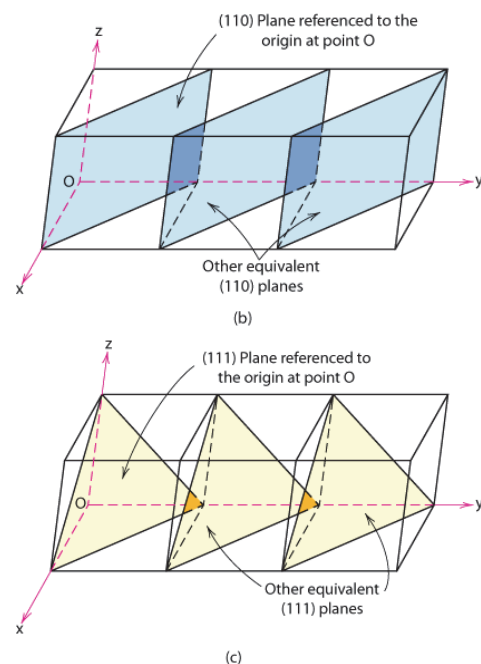
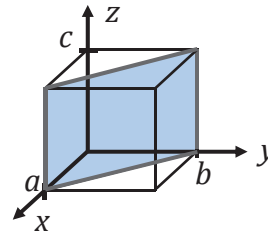


Fig. 3.7 Representation of a series each of the (a) (001) and (b) (110) crystallographic planes.

3.7 Crystallographic Planes

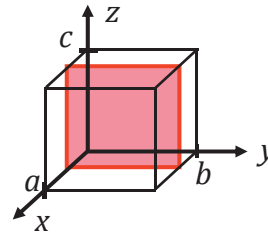
□ Example 1

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



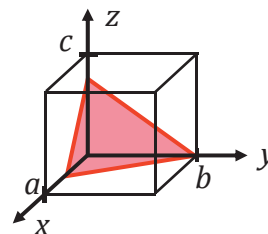
□ Example 2

	a	b	c
1. Intercepts	$\frac{1}{2}$	∞	∞
2. Reciprocals	$1/\frac{1}{2}$	$1/\infty$	$1/\infty$
3. Reduction	2	0	0
4. Miller Indices	(100)		



□ Example 3

	a	b	c
1. Intercepts	$\frac{1}{2}$	1	$\frac{3}{4}$
2. Reciprocals	$1/\frac{1}{2}$	$1/1$	$1/\frac{3}{4}$
3. Reduction	2	1	$\frac{4}{3}$
4. Miller Indices	(634)		



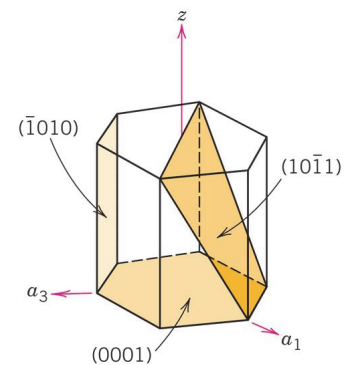
3.7 Crystallographic Planes (HCP)

□ Miller-Bravais system (four axes)

□ Crystallographic Planes (HCP)

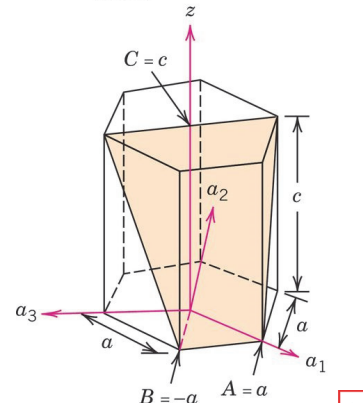
❖ In hexagonal unit cells the same idea is used.

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



□ Example Problem 3.8

	a_1	a_2	a_3	c
1. Intercepts	1	-1	∞	1
2. Reciprocals	1/1	$-1/1$	$1/\infty$	1/1
3. Reduction	1	-1	0	1
4. Miller Indices	$(1\bar{1}01)$			



Crystallographic Point, Direction, & Planar Indices

Table 3.2 Summary of Equations Used to Determine Crystallographic Point, Direction, and Planar Indices

Coordinate Type	Index Symbols	Representative Equation ^a	Equation Symbols
Point	$q\ r\ s$	qa = lattice position referenced to x axis	—
Direction			
Non-hexagonal	$[uvw], [UVW]$	$u = n \left(\frac{x_2 - x_1}{a} \right)$	x_1 = tail coordinate— x axis x_2 = head coordinate— x axis
Hexagonal	$[uvtw]$	$u = 3n \left(\frac{a'_1 - a''_1}{a} \right)$ $u = \frac{1}{3}(2U - V)$	a'_1 = head coordinate— a_1 axis a''_1 = tail coordinate— a_1 axis —
Plane			
Non-hexagonal	(hkl)	$h = \frac{na}{A}$	A = plane intercept— x axis
Hexagonal	$(hkil)$	$i = -(h + k)$	—

^aIn these equations a and n denote, respectively, the x -axis lattice parameter, and a reduction-to-integer parameter.

Crystalline and Noncrystalline Materials

❑ Single Crystals

- ❖ The periodic and repeated arrangement of atoms is perfect or extends throughout the entirety of the specimen without interruption.
- ❖ Examples: Si wafer, GaAs wafer, Al_2O_3 (sapphire) wafer

❑ Polycrystalline Materials

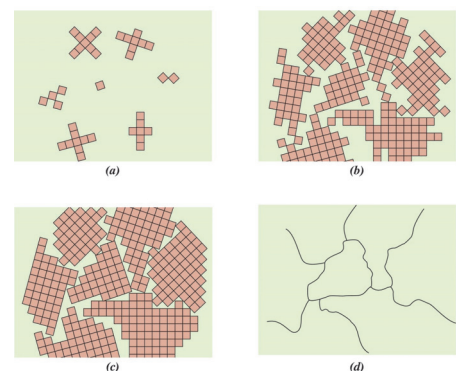
- ❖ A collection of many small crystals or grains

❑ Anisotropy

- ❖ Directionality of material properties
- ❖ For many polycrystalline materials, even though each grain may be anisotropic, a specimen composed of the grain aggregate behaves isotropically.

❑ Noncrystalline (Amorphous) Solids

- ❖ Atomic or molecular structures are relatively complex and become ordered only with some difficulties.
- ❖ Rapidly cooling through the freezing temperature favors the formation of a noncrystalline solid, because little time is allowed for the ordering process.



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

Fig. 3.10 Schematic diagrams of the various stages in the solidification of a polycrystalline material.