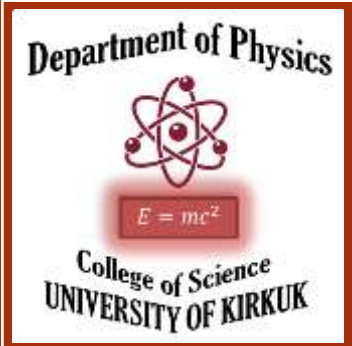



# CRYSTAL SYSTEMS

Subject: Material Science - Lecture #6

مدرسة المادة : الدكتورة روژه برهان الدين عبدالرحمن

Kirkuk University - College of Science

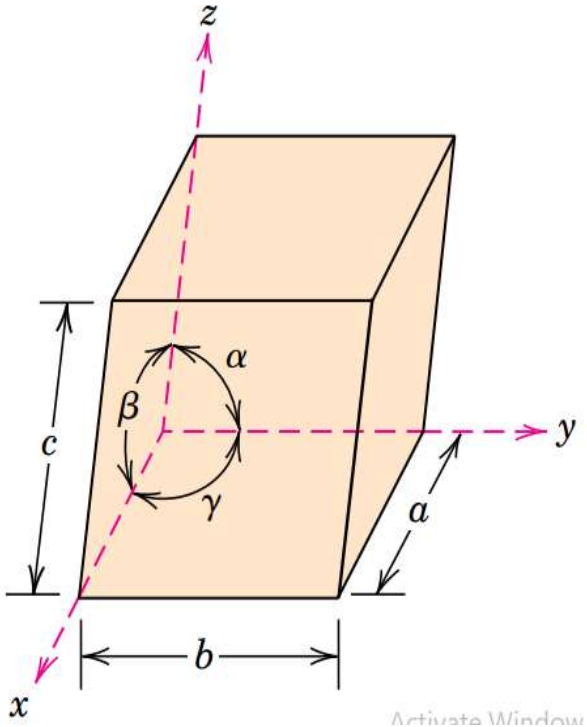
Physics Department – 3rd grade

# CRYSTAL SYSTEMS

- Because there are many different possible crystal structures, it is sometimes convenient to divide them into groups according to unit cell configurations and/or atomic arrangements.

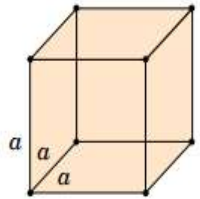
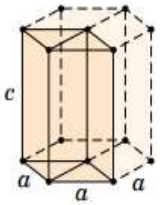
- The scheme which is based on the unit cell geometry, that is, the shape of the appropriate unit cell parallelepiped without regard to the atomic positions in the cell.

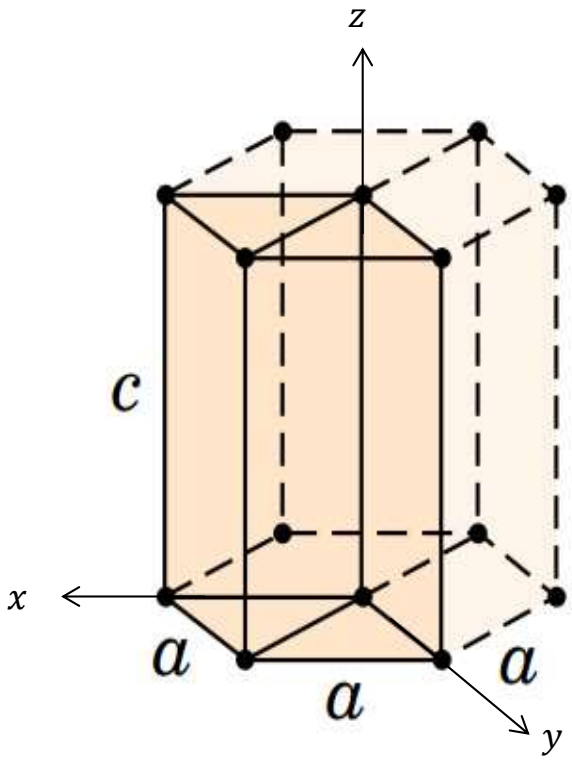
- In the unit cell each of the $x$, $y$, and $z$ axes coincides with one of the three parallelepiped edges that extend from this corner.
- The unit cell geometry is completely defined in terms of six parameters: the three edge lengths $a$, $b$, and $c$, and the three interaxial angles $\alpha$, $\beta$, and $\gamma$. and are sometimes termed the **lattice parameters** of a crystal structure.
- On this basis there are seven different possible combinations of $a$, $b$, and $c$ and $\alpha$, $\beta$, and $\gamma$, each of which represents a distinct **crystal system**.



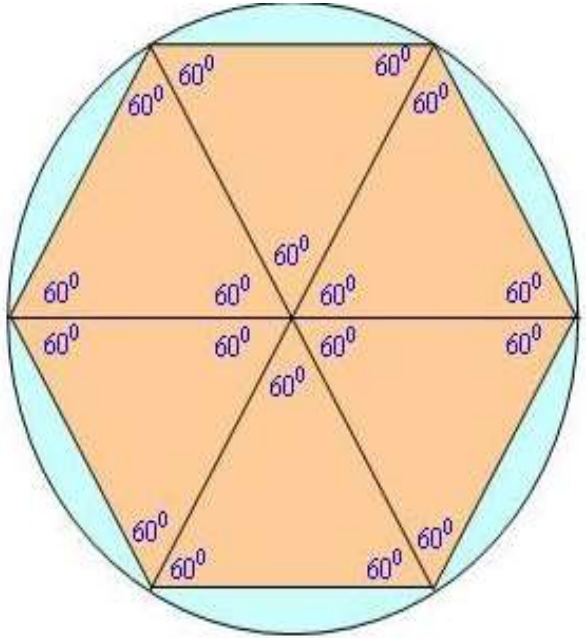
- The seven crystal systems are cubic, tetragonal, hexagonal, orthorhombic, rhombohedral, monoclinic, and triclinic.

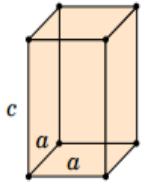
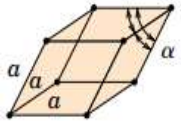
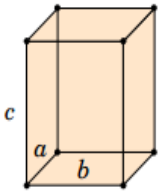
**Table below** show Lattice Parameter Relationships and Figures Showing Unit Cell Geometries for the Seven Crystal Systems

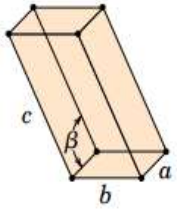
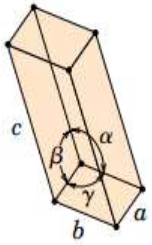
| *Crystal System* | *Axial Relationships* | *Interaxial Angles* | *Unit Cell Geometry* |
|---|---|---|---|
| Cubic | $a = b = c$ | $\alpha = \beta = \gamma = 90^{\circ}$ |   |
| Hexagonal | $a = b \neq c$ | $\alpha = \beta = 90^{\circ}$ $\gamma = 120^{\circ}$ |   |



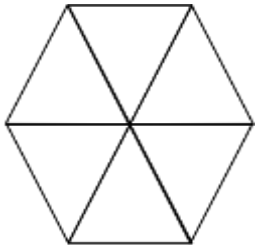

$$\alpha = \beta = 90^{\circ}$$
$$\gamma = 120^{\circ}$$

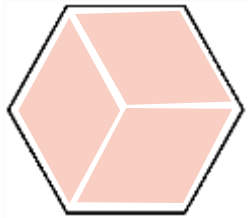


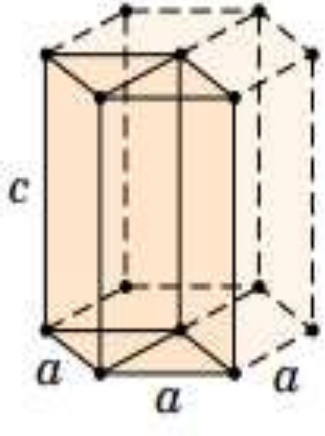
| *Crystal System* | *Axial Relationships* | *Interaxial Angles* | *Unit Cell Geometry* |
|---|---|---|---|
| Tetragonal | $a = b \neq c$ | $\alpha = \beta = \gamma = 90^{\circ}$ |   |
| Rhombohedral (Trigonal) | $a = b = c$ | $\alpha = \beta = \gamma \neq 90^{\circ}$ |   |
| Orthorhombic | $a \neq b \neq c$ | $\alpha = \beta = \gamma = 90^{\circ}$ |   |

| *Crystal System* | *Axial Relationships* | *Interaxial Angles* | *Unit Cell Geometry* |
|---|---|---|---|
| Monoclinic | $a \neq b \neq c$ | $\alpha = \gamma = 90^{\circ} \neq \beta$ |   |
| Triclinic | $a \neq b \neq c$ | $\alpha \neq \beta \neq \gamma \neq 90^{\circ}$ |   |

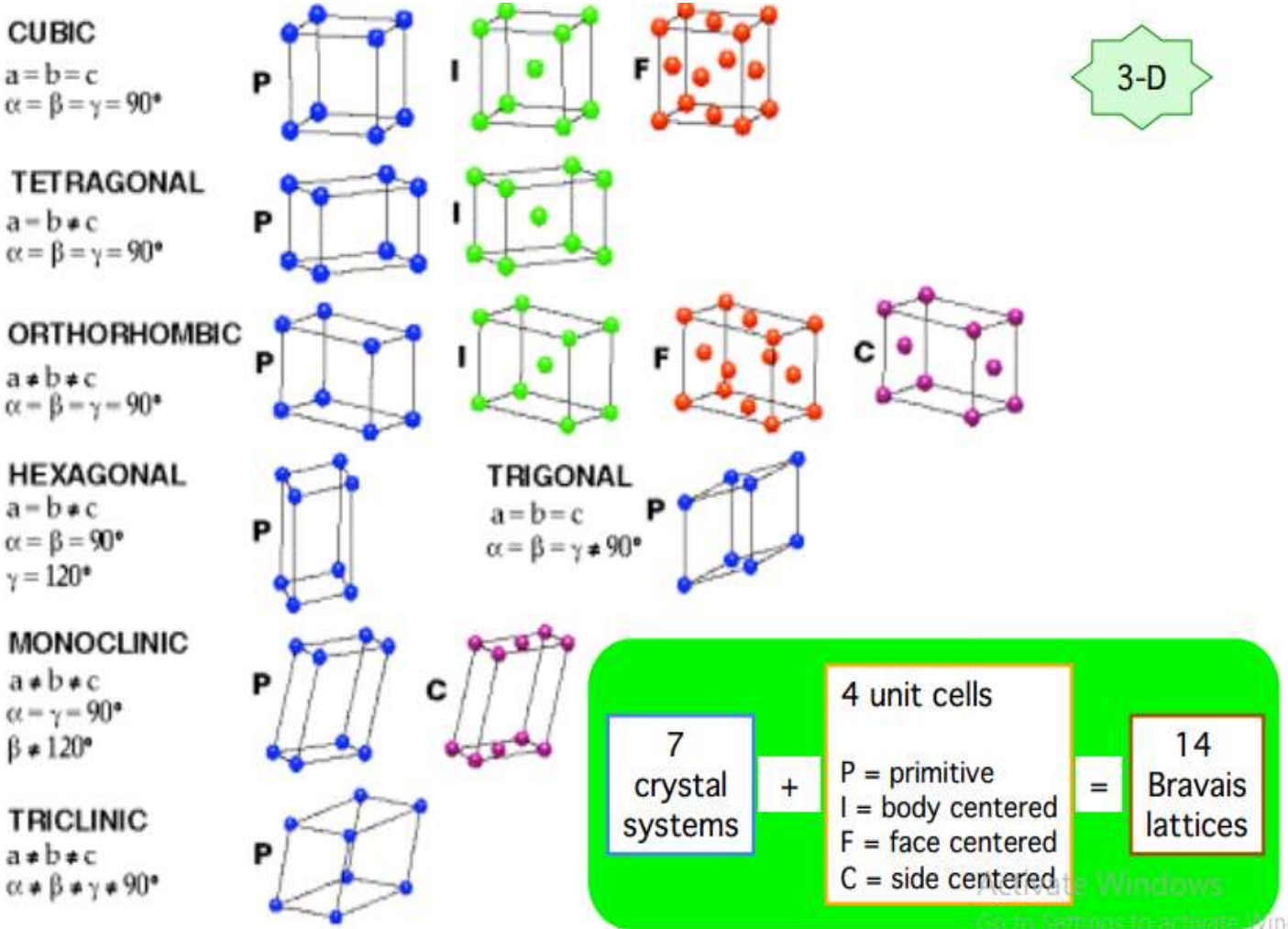
- The cubic system, for which $a = b = c$ and $\alpha = \beta = \gamma = 90^{\circ}$, has the greatest degree of symmetry. The least symmetry is displayed by the triclinic system, because $a \neq b \neq c$ and $\alpha \neq \beta \neq \gamma$.
- Both FCC and BCC structures belong to the cubic crystal system.
- HCP falls within the hexagonal system.
- The conventional hexagonal unit cell consists of three parallelepipeds situated as shown in figure below







- many of the principles and concepts addressed in previous discussions also apply to crystalline ceramic and polymeric systems.
- The crystal structures are most often described in terms of unit cells, which are normally more complex than those for FCC, BCC, and HCP.
- For ceramic and polymeric systems, are often interested in determining atomic packing factors ($APF$) and densities ($\rho$), using modified forms of Equations 3.3 and 3.8.

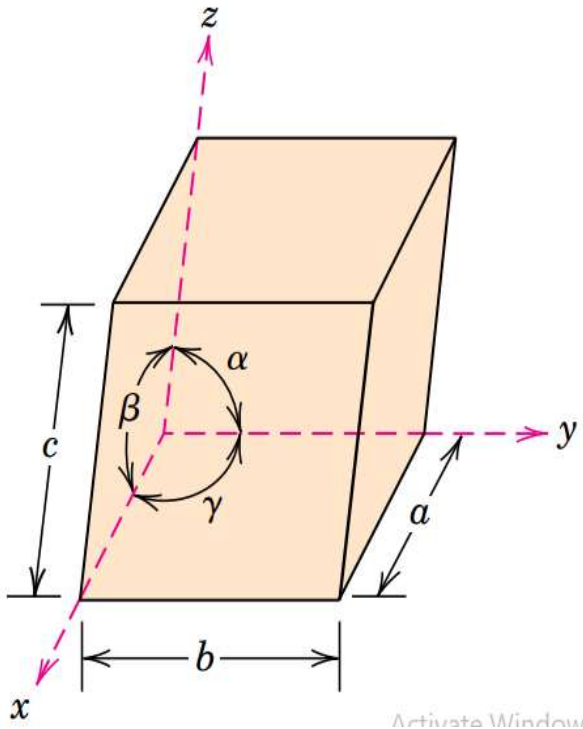

CUBIC
a = b = c
α = β = γ = 90°
P
I
F
3-D
TETRAGONAL
a = b ≠ c
α = β = γ = 90°
P
I
ORTHORHOMBIC
a ≠ b ≠ c
α = β = γ = 90°
P
I
F
C
HEXAGONAL
a = b ≠ c
α = β = 90°
γ = 120°
P
TRIGONAL
a = b = c
α = β = γ ≠ 90°
P
MONOCLINIC
a ≠ b ≠ c
α = γ = 90°
β ≠ 120°
P
C
TRICLINIC
a ≠ b ≠ c
α ≠ β ≠ γ ≠ 90°
P
7 crystal systems
+
4 unit cells
P = primitive
I = body centered
F = face centered
C = side centered
=
14 Bravais lattices

# Crystallographic Points, Directions, and Planes

- When dealing with crystalline materials, it often becomes necessary to specify a particular point within a unit cell, a crystallographic direction, or some crystallographic plane of atoms.

- Labeling conventions have been established in which three numbers or indices are used to designate point locations, directions, and planes.

- The basis for determining index values is the unit cell, with a right-handed coordinate system consisting of three ($x$, $y$, and $z$) axes situated at one of the corners and coinciding with the unit cell edges
- For some crystal systems—namely, hexagonal, rhombohedral, monoclinic, and triclinic—the three axes are *not* mutually perpendicular, as in the familiar Cartesian coordinate scheme.



# POINT COORDINATES

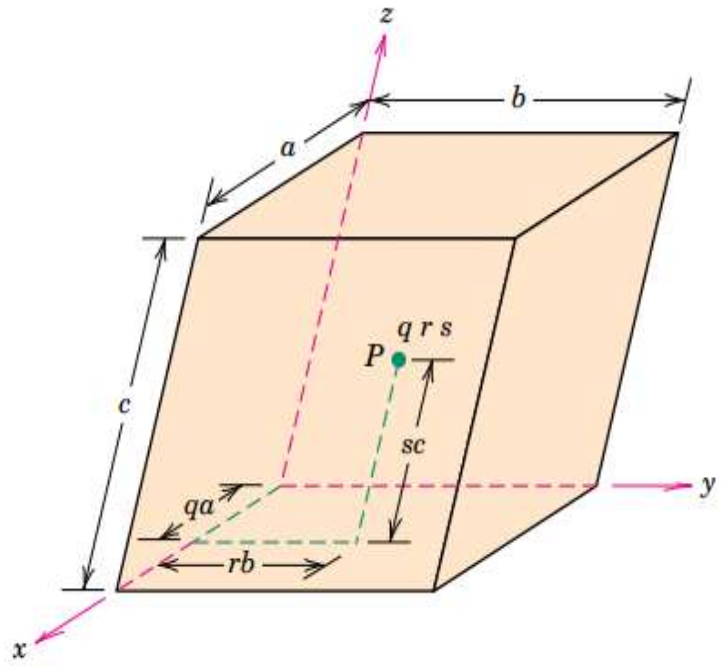
- It is possible to specify a lattice position within a unit cell using three *point coordinate indices*: $q$, $r$, and $s$.
- These indices are fractional multiples of $a$, $b$, and $c$ unit cell edge lengths—that is, $q$ is some fractional length of $a$ along the $x$ axis, $r$ is some fractional length of $b$ along the $y$ axis, and similarly for $s$ ; or

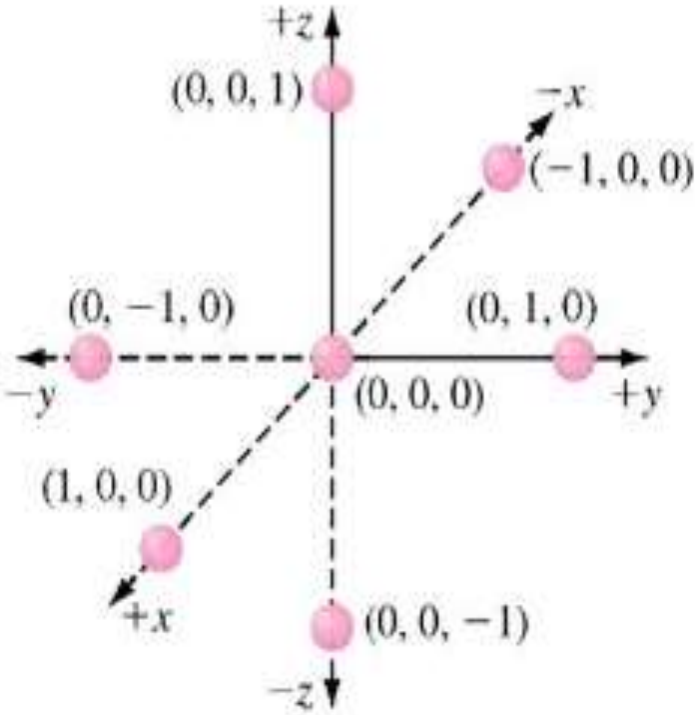
$$qa = \text{lattice position referenced to the } x \text{ axis} \quad \ldots\ldots\ldots (3.9a)$$
$$rb = \text{lattice position referenced to the } y \text{ axis} \quad \ldots\ldots\ldots (3.9b)$$
$$sc = \text{lattice position referenced to the } z \text{ axis} \quad \ldots\ldots\ldots (3.9c)$$

To illustrate a lattice position within a unit cell:

- consider the unit cell in Figure below the $x - y - z$ coordinate system with its origin located at a unit cell corner
- the lattice site located at point $P$.

- The location of $P$ is related to the products of its $q$, $r$, and $s$ coordinate indices and the unit cell edge lengths



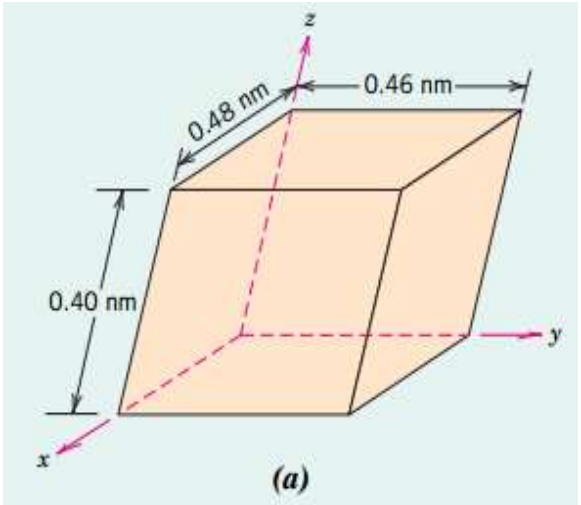

+z
(0, 0, 1)
−x
(−1, 0, 0)
(0, −1, 0)
(0, 1, 0)
−y
(0, 0, 0)
+y
(1, 0, 0)
+x
(0, 0, −1)
−z

# EXAMPLE
# Location of Point Having Specified Coordinates

- For the unit cell shown in the accompanying sketch (*a*), locate the point having coordinates $\frac{1}{4}\,1\,\frac{1}{2}$

***Solution***

From sketch (a), edge lengths for this unit cell are as follows: $a = 0.48\,nm$, $b = 0.46\,nm$, and $c = 0.40\,nm$.
We use Equations 3.9a through 3.9c

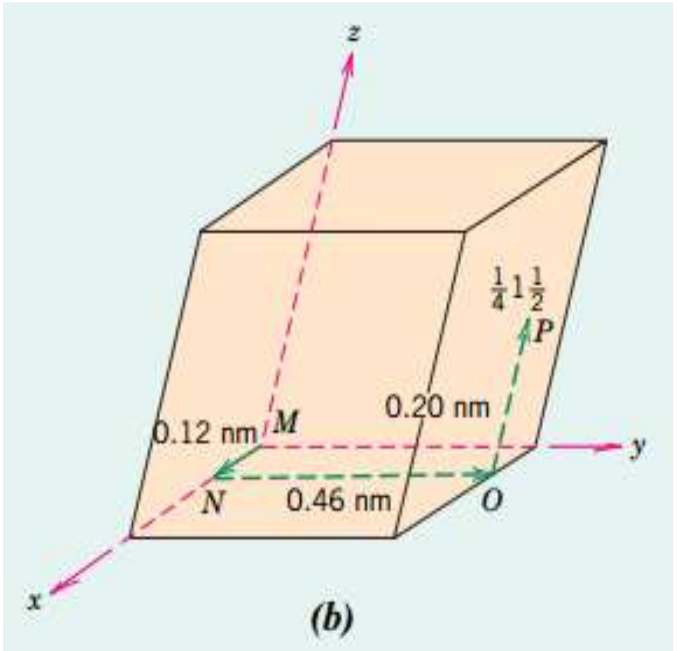


$qa$ = lattice position referenced to the $x$ axis ... ... ... $(3.9a)$
$rb$ = lattice position referenced to the $y$ axis ... ... ... $(3.9b)$
$sc$ = lattice position referenced to the $z$ axis ... ... ... $(3.9c)$

$$qa = (\frac{1}{4})a = \frac{1}{4}(0.48\ nm) = 0.12\ nm$$

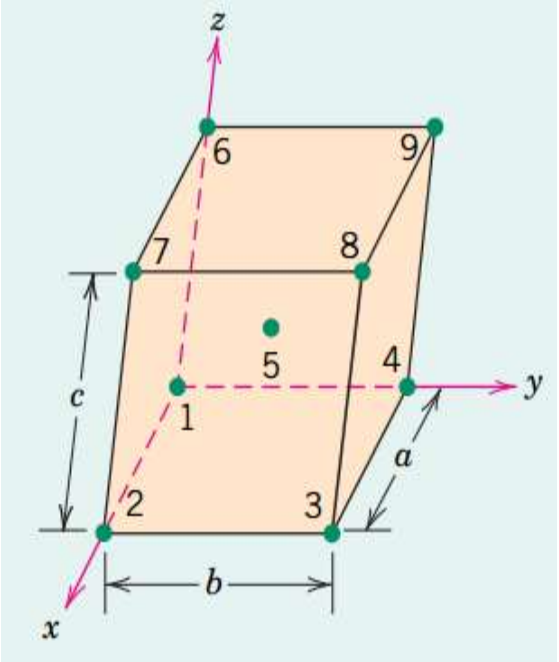
$$rb = (1)b = (1)(0.46\ nm) = 0.46\ \text{nm}$$

$$sc = (\frac{1}{2})c = \frac{1}{2}(0.40\ nm) = 0.20\ nm$$



# EXAMPLE
# Specification of Point Coordinate Indices

Specify coordinate indices for all numbered points of the unit cell in the Figure below.



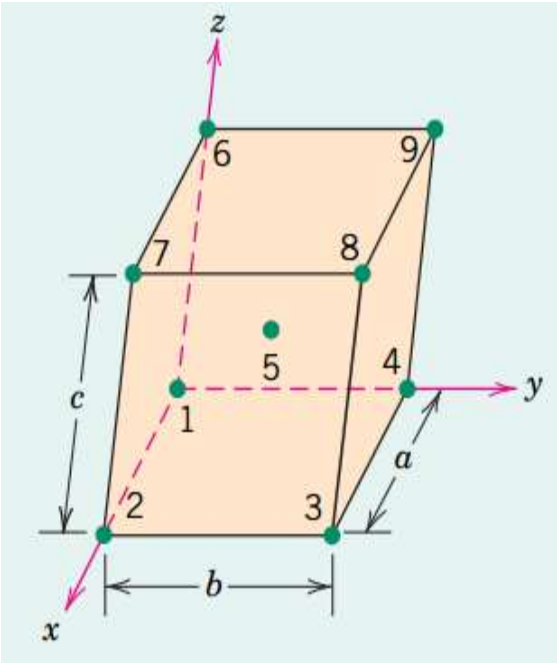

***Solution***

$qa$ = lattice position referenced to the $x$ axis ... ... ... $(3.9a)$
$rb$ = lattice position referenced to the $y$ axis ... ... ... $(3.9b)$
$sc$ = lattice position referenced to the $z$ axis ... ... ... $(3.9c)$

- Point 1 is located at the origin of the coordinate system
  lattice position referenced to the $x$ axis $= 0a = qa$
  $lattice\ position\ referenced\ to\ the\ y$ axis $= 0b = rb$
  lattice position referenced to the $z$ axis $= 0c = sc$
  Solving the above three expressions for values of the $q$, $r$, and $s$ indices leads to

$$q = \frac{0a}{a} = 0 \quad ; \quad r = \frac{0b}{b} = 0 \quad ; \quad s = \frac{0c}{c} = 0$$

Therefore this is the 0 0 0 point



# CRYSTALLOGRAPHIC DIRECTIONS

A ***crystallographic direction*** is defined as a line directed between two points, or a *vector*.

The following steps are used to determine the three directional indices:

**1.** A right-handed $x - y - z$ coordinate system is first constructed. As a matter of convenience, its origin may be located at a unit cell corner.

**2.** The coordinates of two points that lie on the direction vector (referenced to the coordinate system) are determined - for example, for the vector tail, point 1: $x_1, y_1$ and $z_1$; whereas for the vector head, point 2: $x_2, y_2$ and $z_2$.

**3.** Tail point coordinates are subtracted from head point components—that is, $x_2 - x_1, y_2 - y_1$ and $z_2 - z_1$

**4.** These coordinate differences are then normalized in terms of (i.e., divided by) their respective $a$, $b$, and $c$ lattice parameters—that is,

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

which yields a set of three numbers.

**5.** If necessary, these three numbers are multiplied or divided by a common factor to reduce them to the smallest integer values.

**6.** The three resulting indices, not separated by commas, are enclosed in square brackets, thus: $[uvw]$. The $u$, $v$, and $w$ integers correspond to the normalized coordinate differences referenced to the $x$, $y$, and $z$ axes, respectively.

In summary, the $u$, $v$, and $w$ indices may be determined using the following equations:

$$u = n\left(\frac{x_2 - x_1}{a}\right) \quad \ldots\ldots\ldots\ldots (3.10a)$$

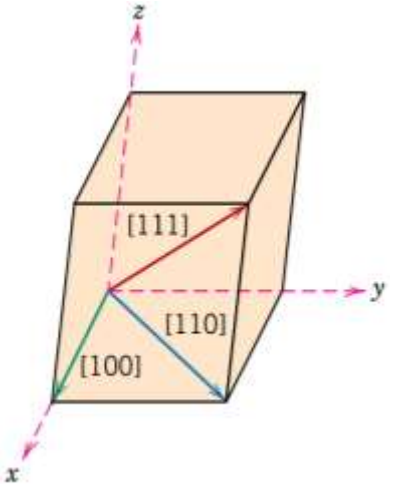
$$v = n\left(\frac{y_2 - y_1}{b}\right) \quad \ldots\ldots\ldots\ldots (3.10b)$$

$$w = n\left(\frac{z_2 - z_1}{c}\right) \quad \ldots\ldots\ldots\ldots (3.10c)$$

In these expressions, $n$ is the factor that may be required to reduce $u$, $v$, and $w$ to integers.

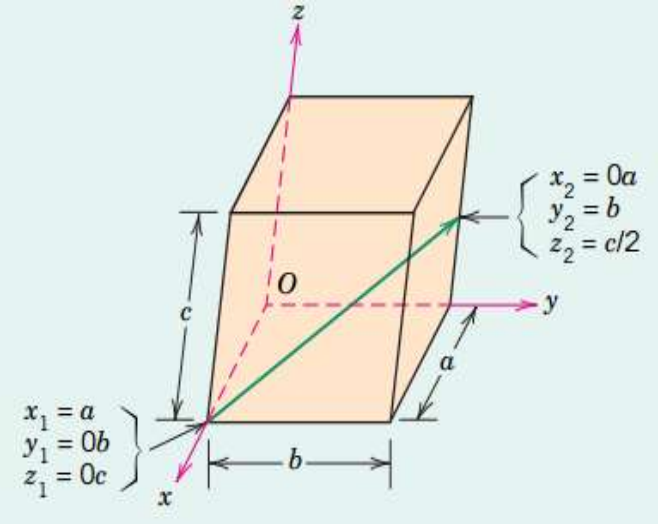
- For each of the three axes, there are both positive and negative coordinates. which are represented by a bar over the appropriate index. For example, the $[1\bar{1}1]$ direction has a component in the $-y$ direction.
- Also, changing the signs of all indices produces an antiparallel direction; that is, $[\bar{1}1\bar{1}]$ is directly opposite to $[1\bar{1}1]$ .

- The $[100]$, $[110]$, and $[111]$ directions are common ones; they are drawn in the unit cell shown in Figure.



# EXAMPLE
# Determination of Directional Indices

Determine the indices for the direction shown in the accompanying figure.



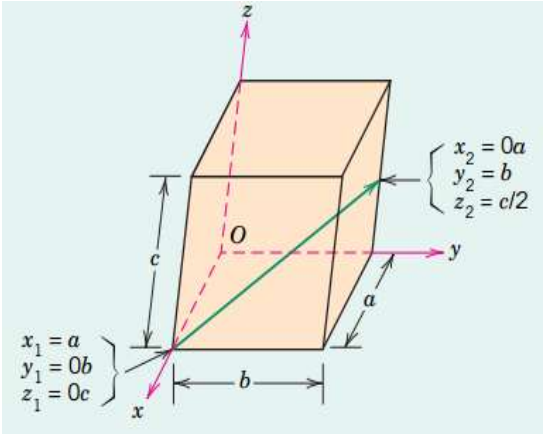
***Solution***

the tail coordinates,

$x_1 = a \qquad y_1 = 0b \qquad z_1 = 0c$

For the head coordinates,

$x_2 = 0a \qquad y_2 = b \qquad z_2 = c/2$




Now taking point coordinate differences,

$x_2 - x_1 = 0a - a = -a$ (integers)

$y_2 - y_1 = b - 0b = b$ (integers)

$z_2 - z_1 = \frac{c}{2} - 0c = \frac{c}{2}$ (fraction)

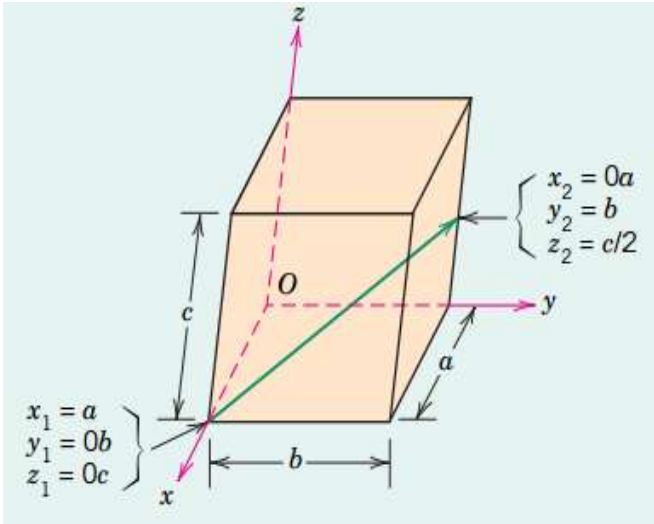
to compute values of $u$, $v$, and $w$ we use Equations 3.10a through 3.10c

in order to have integer values for the three indices, it is necessary to assign $n$ a value of 2. Thus,

$$u = n\left(\frac{x_2 - x_1}{a}\right) = 2\left(\frac{-a}{a}\right) = -2$$

$$v = n\left(\frac{y_2 - y_1}{b}\right) = 2\left(\frac{b}{b}\right) = 2$$

$$w = n\left(\frac{z_2 - z_1}{c}\right) = 2\left(\frac{c}{2}\right) = 1$$

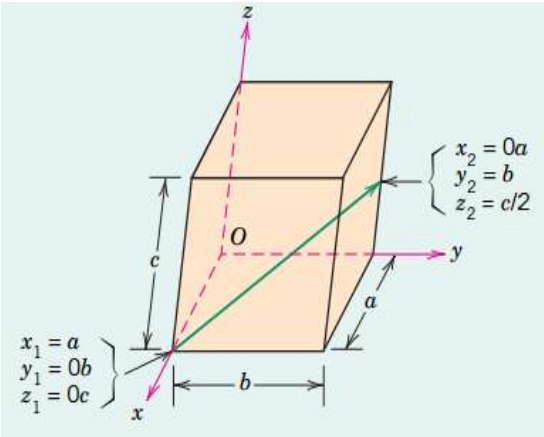



finally enclosure of the -2, 2, and 1 indices in brackets of form $[uvw]$ leads to $[221]$ as the direction designation.

If these $u, v,$ and $w$ values are not integers, it is necessary to choose another value for $n$.

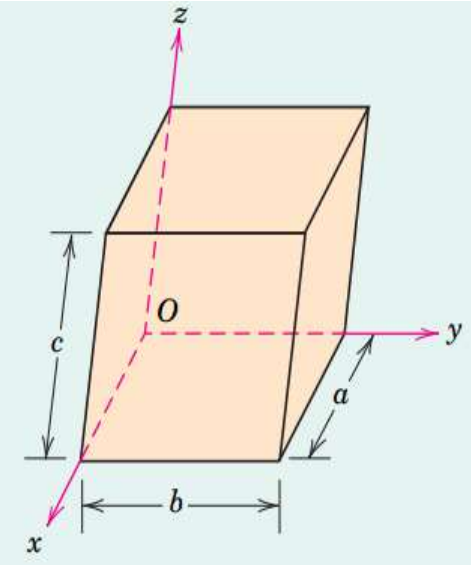
This procedure is summarized as follows:

| | *x* | *y* | *z* |
|---|---|---|---|
| Head coordinates ($x_2$, $y_2$, $z_2$,) | $0a$ | $b$ | $c/2$ |
| Tail coordinates ($x_1$, $y_1$, $z_1$,) | $a$ | $0b$ | $0c$ |
| Coordinate differences | $-a$ | $b$ | $c/2$ |
| Calculated values of $u$, $v$, and $w$ | $u = -2$ | $v = 2$ | $w = 1$ |
| Enclosure | | $[\bar{2}21]$ | |



# EXAMPLE
# Construction of a Specified Crystallographic Direction

Within the following unit cell draw a $[1\bar{1}0]$ direction with its tail located at the origin of the coordinate system, point *O*.



***Solution***

This problem is solved by reversing the procedure of the preceding example.

For this $[1\bar{1}0]$ direction,

$u = 1$

$v = -1$

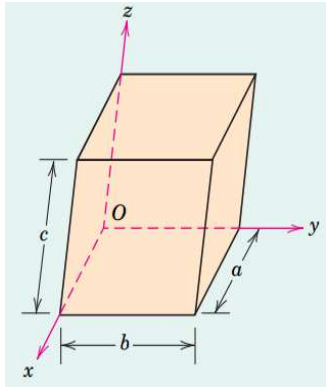
$w = 0$

Because the tail of the direction vector is positioned at the origin, its coordinates are as follows:

$x_1 = 0a$

$y_1 = 0b$

$z_1 = 0c$

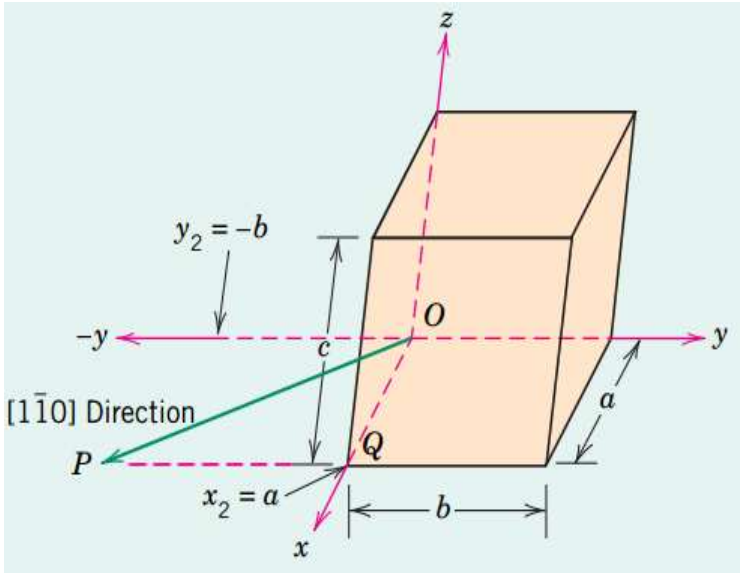


We now want to solve for the coordinates of the vector head—that is, $x_2, y_2$ and $z_2$.

By using rearranged forms of Equations 3.10a through 3.10c

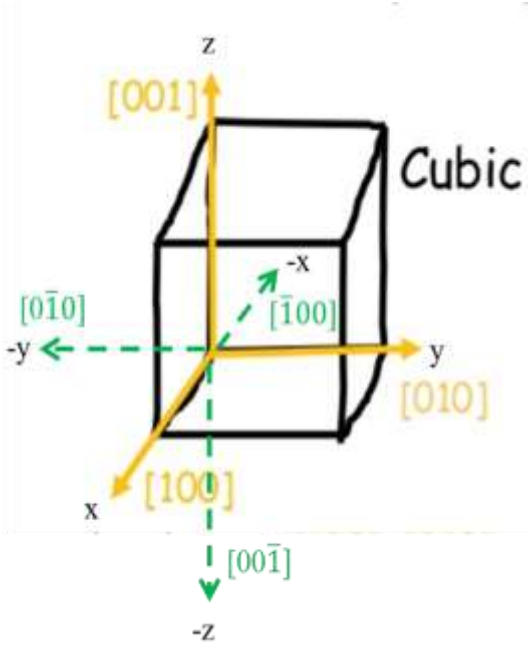
$$x_2 = ua + x_1 = (1)(a) + 0a = a$$
$$y_2 = vb + y_1 = (-1)(b) + 0b = -b$$
$$z_2 = wc + z_1 = (0)(c) + 0c = 0c$$

the vector corresponding to this $[1\bar{1}0]$ direction is constructed by drawing a line from point O to point P



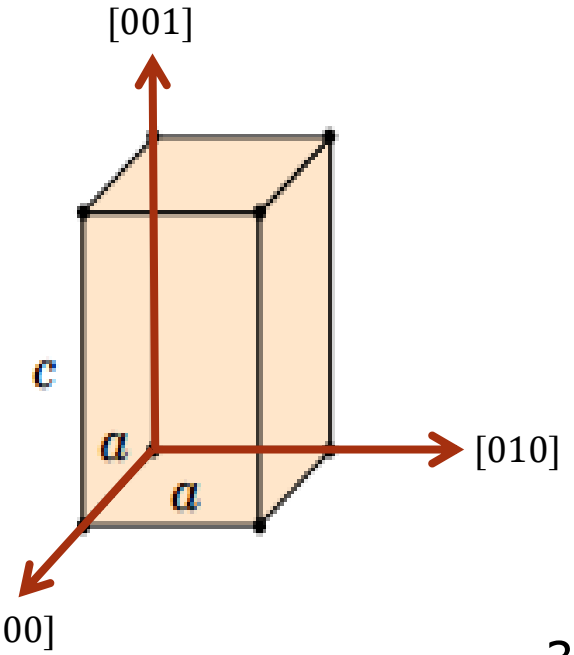
- For some crystal structures, several nonparallel directions with different indices are *crystallographically equivalent*, meaning that the spacing of atoms along each direction is the same.

- For example, in cubic crystals, all the directions represented by the following indices are equivalent: $[100], [\bar{1}00], [010], [0\bar{1}0], [001], \text{and } [00\bar{1}]$.
- Equivalent directions are grouped together into a family, which is enclosed in angle brackets, thus: $< 100 >$.



- directions in cubic crystals having the same indices without regard to order or sign—for example, $[123]$ and $[\bar{2}1\bar{3}]$—are equivalent.

- This is, in general, not true for other crystal systems. For example, for crystals of tetragonal symmetry, the $[100]$ and $[010]$ directions are equivalent, whereas the $[100]$ and $[001]$ are not.



Thank you for your attention

?