Material Science
The Structure of Solids:
Crystal System, Crystal Directions (Weeks 6)

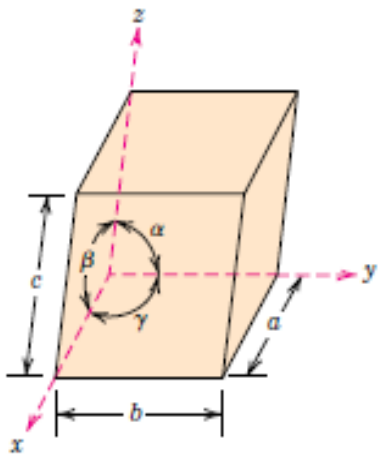
Presented by Professor Ali Hussein Ataiwi

CRYSTAL SYS

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. One such scheme 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. Within this framework, an xyz coordinate system is established with its origin at one of the unit cell corners; each of the x, y, and z axes coincides with one of the three parallelepiped edges that extend from this corner, as illustrated in Figure 3.5. The unit cell geometry is completely defined in terms of six parameters: the three edge lengths a, b, and c, and the three inter axial angles α, β, and γ. These are indicated in Figure 3.5, 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 α, β, and γ. each of which represents a distinct crystal system.

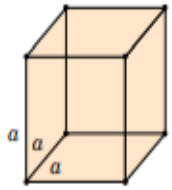
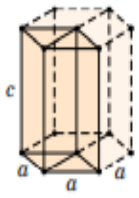
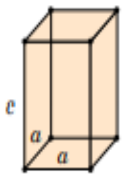
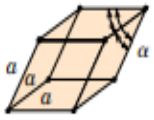
Figure 3.5 A unit cell with x, y, and z coordinate axes, showing axial lengths (a, b, and c) and interaxial angles (α, β, and γ).



The lattice parameter relationships and unit cell sketches for each are represented in Table 3.2. The cubic system, for which $a = b = c$ and $\alpha = \beta = \gamma = 90°$, has the greatest degree of symmetry. The least symmetry is displayed by the triclinic system, because $a \neq b \neq c$ and $\alpha \neq \beta \neq \gamma$. From the discussion of metallic crystal structures, it should be apparent that both FCC and BCC structures belong to the cubic crystal system, whereas HCP falls within the hexagonal system. The conventional hexagonal unit cell really consists of three parallelepipeds situated as shown in Table 3.2.

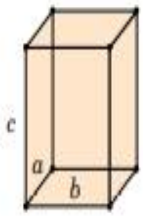
It is important to note that many of the principles and concepts addressed in previous discussions in this chapter also apply to crystalline ceramic and polymeric systems.

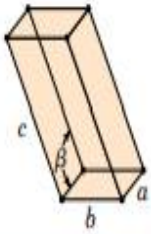
Table 3.2 Lattice Parameter Relationships and Figures Showing Unit Cell Geometries for the Seven Crystal Systems

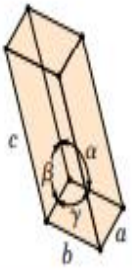
Crystal System	Axial Relationships	Interaxial Angles	Unit Cell Geometry
Cubic	$a = b = c$	$\alpha = \beta = \gamma = 90°$	
Hexagonal	$a = b \neq c$	$\alpha = \beta = 90°, \gamma = 120°$	
Tetragonal	$a = b \neq c$	$\alpha = \beta = \gamma = 90°$	
Rhombohedral (Trigonal)	$a = b = c$	$\alpha = \beta = \gamma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

WileyPLUS: VMSE
Crystal Systems and Unit Cells for Metals

	Orthorhombic	$a \neq b \neq c$	$\alpha = \beta = \gamma = 90^\circ$
	Monoclinic	$a \neq b \neq c$	$\alpha = \gamma = 90^\circ \neq \beta$
	Triclinic	$a \neq b \neq c$	$\alpha \neq \beta \neq \gamma \neq 90^\circ$







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. Labelling 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, as shown in Figure 3.5. For some crystal systems—namely, hexagonal, rhombohedral, monoclinic, and triclinic—the three axes are not mutually perpendicular, as in the familiar Cartesian coordinate scheme.

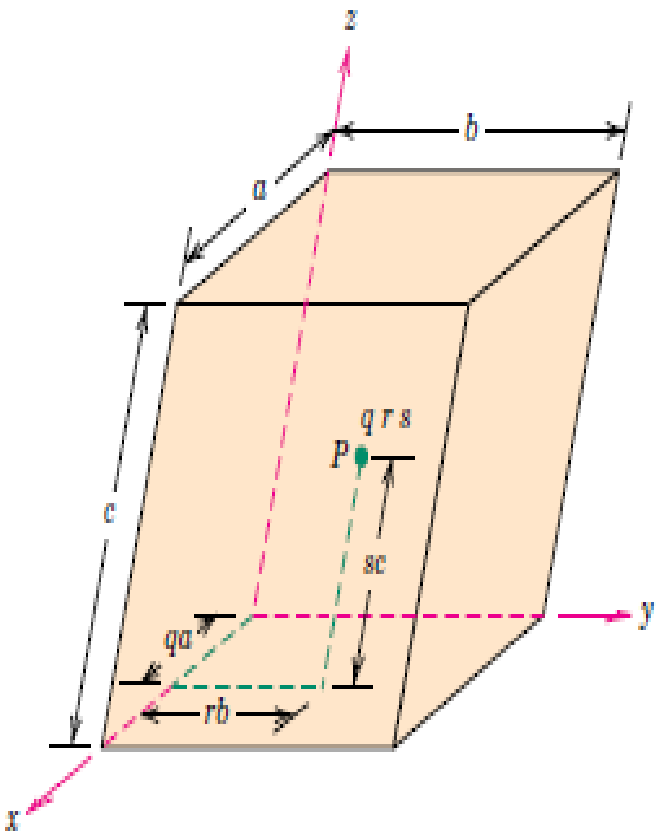
3.8 POINT COORDINATE

Sometimes it is necessary to specify a lattice position within a unit cell. This is possible 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 = 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)

To illustrate, consider the unit cell in Figure 3.6, the x-y-z coordinate system with its origin located at a unit cell corner, and the lattice site located at point P. Note how the location of P is related to the products of its q, r, and s coordinate indices and the unit cell edge lengths.

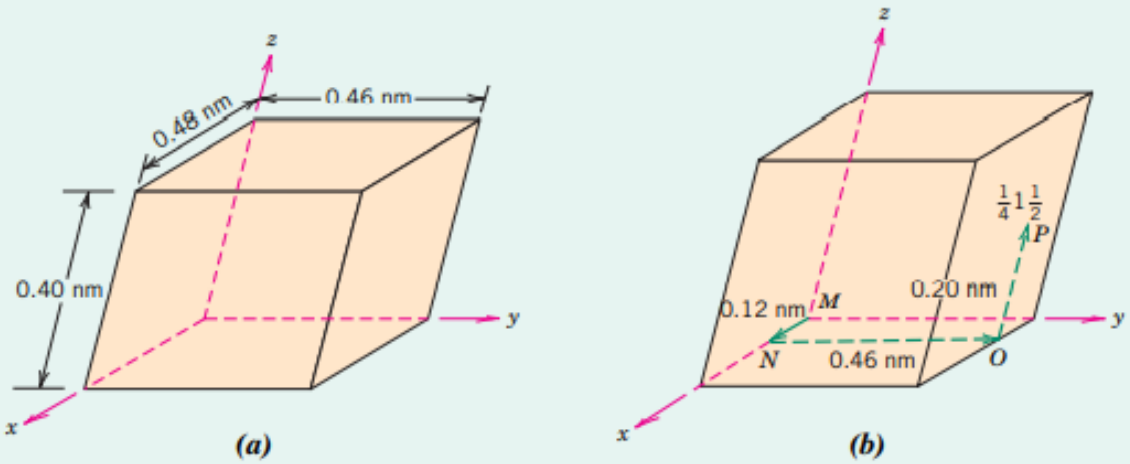
Figure 3.6 The manner in which the *q*, *r*, and *s* coordinates at point *P* within the unit cell are determined. The *q* coordinate (which is a fraction) corresponds to the distance *qa* along the *x* axis, where *a* is the unit cell edge length. The respective *r* and *s* coordinates for the y and *z* axes are determined similarly.



EXAMPLE PROBLEM 3.5

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. Furthermore, in light of the preceding discussion, the three point coordinate indices are $q = \frac{1}{4}$, $r = 1$, and $s = \frac{1}{2}$. We use Equations 3.9a through 3.9c to determine lattice positions for this point as follows:

$$\text{lattice position referenced to the } x \text{ axis} = qa$$
$$= \left(\tfrac{1}{4}\right)a = \tfrac{1}{4}(0.48\text{ nm}) = 0.12\text{ nm}$$

$$\text{lattice position referenced to the } y \text{ axis} = rb$$
$$= (1)b = (1)(0.46\text{ nm}) = 0.46\text{ nm}$$

$$\text{lattice position referenced to the } z \text{ axis} = sc$$
$$= \left(\tfrac{1}{2}\right)c = \left(\tfrac{1}{2}\right)(0.40\text{ nm}) = 0.20\text{ nm}$$

To locate the point having these coordinates within the unit cell, first use the *x* lattice position and move from the origin (point *M*) 0.12 nm units along the *x* axis (to point *N*), as shown in (*b*). Similarly, using the *y* lattice position, proceed 0.46 nm parallel to the *y* axis, from point *N* to point *O*. Finally, move from this position 0.20 nm units parallel to the *z* axis to point *P* (per the *z* lattice position), as noted again in (*b*). Thus, point *P* corresponds to the $\frac{1}{4}\,1\,\frac{1}{2}$ point coordinates.

EXAMPLE PROBLEM 3.6

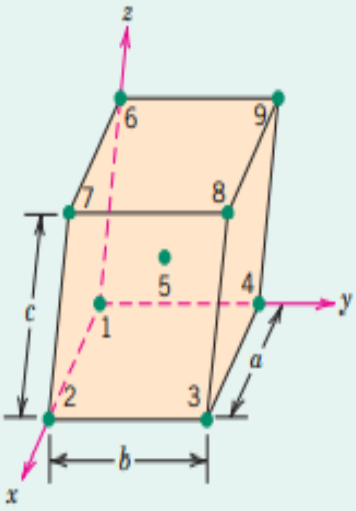
Specification of Point Coordinate Indices

Specify coordinate indices for all numbered points of the unit cell in the illustration shown below

Solution

For this unit cell, coordinate points are located at all eight corners with a single point at the center position.

Point 1 is located at the origin of the coordinate system, and, therefore, its lattice position indices referenced to the x, y, and z axes are $0a$, $0b$, and $0c$, respectively. And from Equations 3.9a through 3.9c,



$$\text{lattice position referenced to the } x \text{ axis} = 0a = qa$$

$$\text{lattice position referenced to the } y \text{ axis} = 0b = rb$$

$$\text{lattice position referenced to the } z \text{ axis} = 0c = sc$$

Solving the above three expressions for values of the q, r, and s indices leads to

$$q = \frac{0a}{a} = 0$$

$$r = \frac{0b}{b} = 0$$

$$s = \frac{0c}{c} = 0$$

Therefore this is the 0 0 0 point

Because point number 2, lies one unit cell edge length along the x axis, its lattice position indices referenced to the x, y, and z axes are a, $0b$, and $0c$, and

$$\text{lattice position index referenced to the } x \text{ axis} = a = qa$$

$$\text{lattice position index referenced to the } y \text{ axis} = 0b = rb$$

$$\text{lattice position index referenced to the } z \text{ axis} = 0c = sc$$

Thus we determine values for the q, r, and s indices as follows:

$$q = 1 \qquad r = 0 \qquad s = 0$$

Hence, point 2 is 1 0 0.

This same procedure is carried out for the remaining seven points in the unit cell. Point indices for all nine points are listed in the following table.

Point Number	*q*	*r*	*s*
1	0	0	0
2	1	0	0
3	1	1	0
4	0	1	0
5	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$
6	0	0	1
7	1	0	1
8	1	1	1
9	0	1	1

3.9 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:

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

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

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

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. Thus, negative indices are also possible, 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]. If more than one direction (or plane) is to be specified for a particular crystal structure, it is imperative for maintaining consistency that a positive–negative convention, once established, not be changed.

The [100], [110], and [111] directions are common ones; they are drawn in the unit cell shown in Figure 3.7.

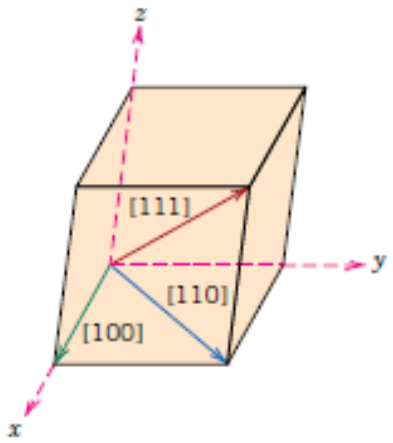


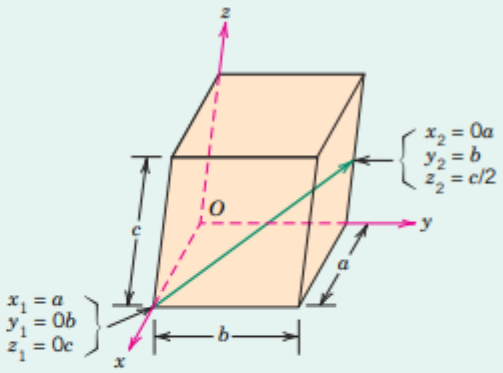
Figure 3.7 The [100], [110], and [111] directions within a unit cell.

Note: The directions in hexagonal crystals are outside of the scope of discussion in second year

EXAMPLE PROBLEM 3.7

Determination of Directional Indices

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



Solution

It is first necessary to take note of the vector tail and head coordinates. From the illustration, tail coordinates are as follows:

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

For the head coordinates,

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

Now taking point coordinate differences,

$$x_2 - x_1 = 0a - a = -a$$
$$y_2 - y_1 = b - 0b = b$$
$$z_2 - z_1 = c/2 - 0c = c/2$$

It is now possible to use Equations 3.10a through 3.10c to compute values of u, v, and w. However, because the $z_2 - z_1$ difference is a fraction (i.e., $c/2$), we anticipate that in order to have integer values for the three indices, it is necessary to assign n a value of 2. Thus,

$$u = n\left(\frac{x_2 - x_1}{a}\right) = 2\left(\frac{-a}{a}\right) = -2$$
$$v = n\left(\frac{y_2 - y_1}{b}\right) = 2\left(\frac{b}{b}\right) = 2$$
$$w = n\left(\frac{z_2 - z_1}{c}\right) = 2\left(\frac{c/2}{c}\right) = 1$$

And, finally enclosure of the −2, 2, and 1 indices in brackets leads to $[\bar{2}21]$ as the direction designation.[4]

This procedure is summarized as follows:

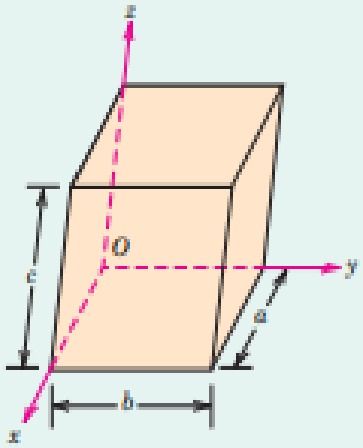
	x	y	z
Head coordinates (x_2, y_2, z_2)	$0a$	b	$c/2$
Tail coordinates (x_1, y_1, z_1)	a	$0b$	$0c$
Coordinate differences	$-a$	b	$c/2$
Calculated values of u, v, and w	$u = -2$	$v = 2$	$w = 1$
Enclosure		$[\bar{2}21]$	

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

EXAMPLE PROBLEM 3.8

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,

$$u = 1$$
$$v = -1$$
$$w = 0$$

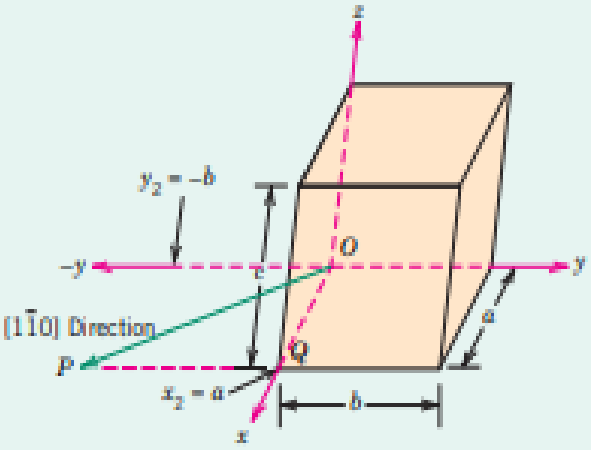
Because the tail of the direction vector is positioned at the origin, its coordinates are as follows:

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

We now want to solve for the coordinates of the vector head—that is, x_2, y_2, and z_2. This is possible using rearranged forms of Equations 3.10a through 3.10c and incorporating the above values for the three direction indices (u, v, and w) and vector tail coordinates. Taking the value of n to be 1 because the three direction indices are all integers leads to

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

The construction process for this direction vector is shown in the following figure.



Because the tail of the vector is positioned at the origin, we start at the point labeled O and then move in a stepwise manner to locate the vector head. Because the x head coordinate (x_2) is a, we proceed from point O, a units along the x axis to point Q. From point Q, we move b units parallel to the $-y$ axis to point P, because the y head coordinate (y_2) is $-b$. There is no z component to the vector inasmuch as the z head coordinate (z_2) is $0c$. Finally, the vector corresponding to this $[1\bar{1}0]$ direction is constructed by drawing a line from point O to point P, as noted in the illustration.