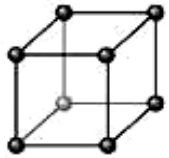
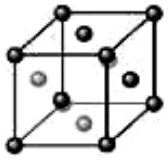
Lattice, Unit Cells, Basis, and Crystal Structures

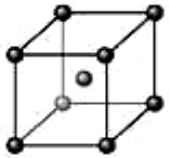
- Lattice - a 3D collection of points that divide space into smaller equally sized units.
- Basis - a group of atoms associated with a lattice point. This may be one single atom or a group of atoms.
- Unit cell - a subdivision of the lattice that still retains the overall characteristics of the entire lattice, contains at least one atom may contain many atoms.
- Atomic radius - apparent radius of an atom, typically calculated from the dimensions of the unit cell, using close-packed directions (depends upon type of bonding, coordination number, quantum mechanics).
- Packing factor - The fraction of space in a unit cell occupied by atoms.



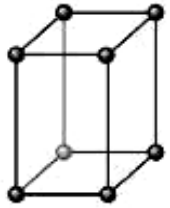
Simple cubic



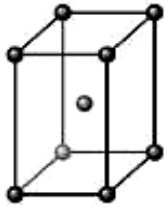
Face-centered cubic



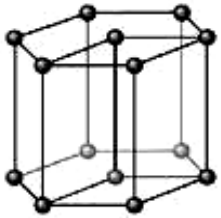
Body-centered cubic



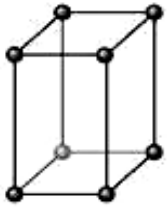
Simple tetragonal



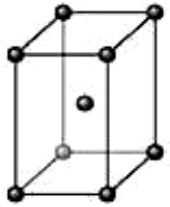
Body-centered tetragonal



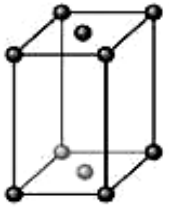
Hexagonal



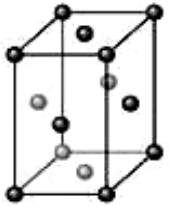
Simple orthorhombic



Body-centered orthorhombic

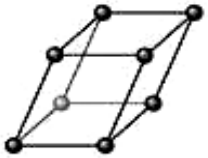


Base-centered orthorhombic

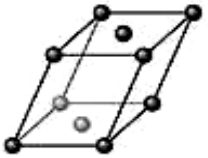


Face-centered orthorhombic

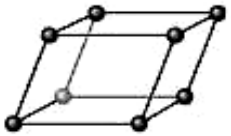
Rhombohedral



Simple monoclinic



Base-centered monoclinic



Triclinic

The fourteen types of Bravais) lattices grouped in seven crystal systems:

triclinic

monocline

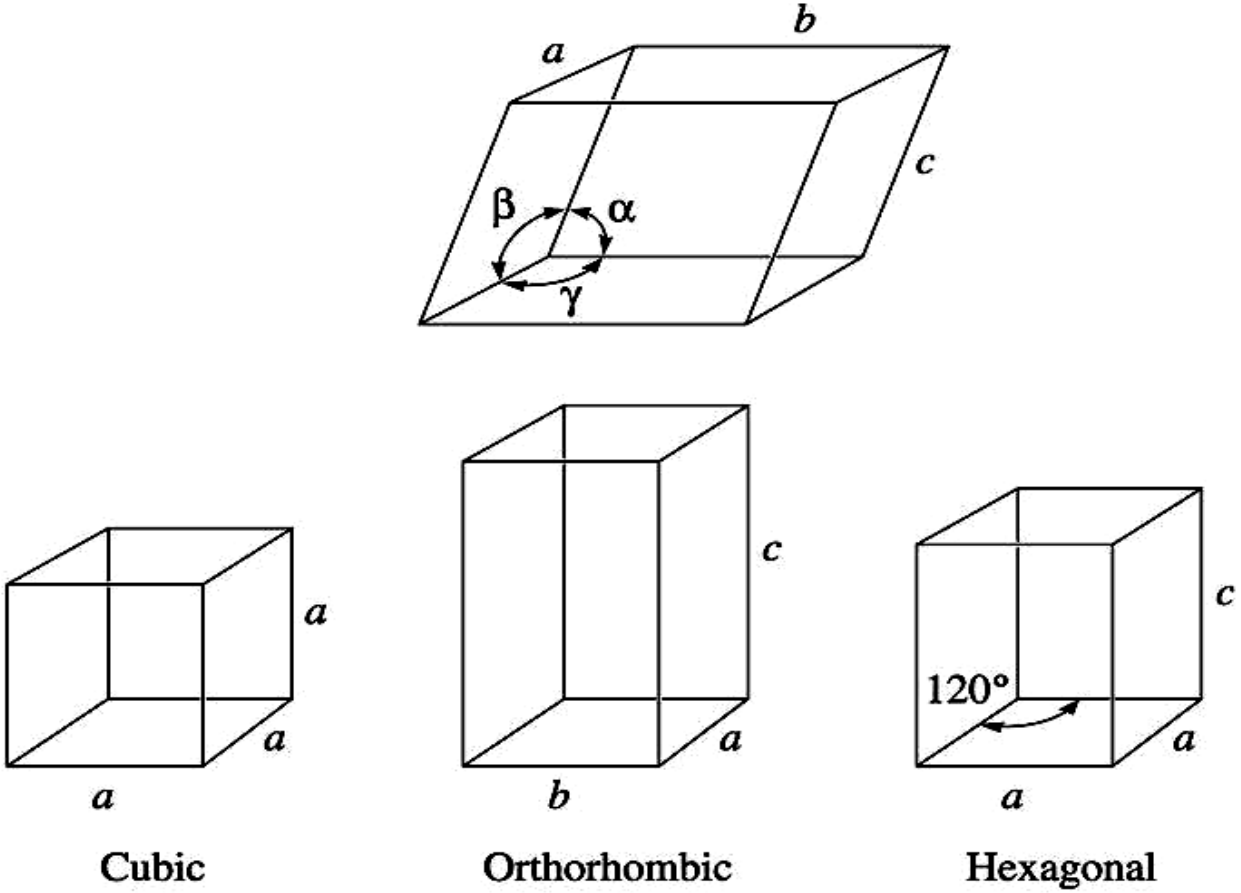
rhombohedral = (trigonal)

orthorhombic

tetragonal

hexagonal

cubic



Definition of lattice parameters in cubic, orthorhombic, and hexagonal crystal systems.

Note that angles are not always 90° degrees and coordination axis lengths are not necessarily all equal, as you know them to be from Cartesian coordinates

For cubic crystals, however, calculations are just like with Cartesian coordinates

TABLE 3-1 ■ *Characteristics of the seven crystal systems*

Structure	Axes	Angles between Axes	Volume of the Unit Cell
Cubic	$a = b = c$	All angles equal 90°	a^3
Tetragonal	$a = b \neq c$	All angles equal 90°	a^2c
Orthorhombic	$a \neq b \neq c$	All angles equal 90°	abc
Hexagonal	$a = b \neq c$	Two angles equal 90°. One angle equals 120°.	$0.866a^2c$
Rhombohedral or trigonal	$a = b = c$	All angles are equal and none equals 90°	$a^3\sqrt{1 - 3\cos^2\alpha + 2\cos^3\alpha}$
Monoclinic	$a \neq b \neq c$	Two angles equal 90°. One angle (β) is not equal to 90°	$abc \sin\beta$
Triclinic	$a \neq b \neq c$	All angles are different and none equals 90°	$abc\sqrt{1 - \cos^2\alpha - \cos^2\beta - \cos^2\gamma + 2\cos\alpha\cos\beta\cos\gamma}$

Lattice Points and Directions in the Unit Cell

- Miller-indices - A shorthand notation to describe certain crystallographic directions and planes in a material.

Lattice directions are in direct space and are denoted by [ ] brackets. A negative number is represented by a bar over the number.

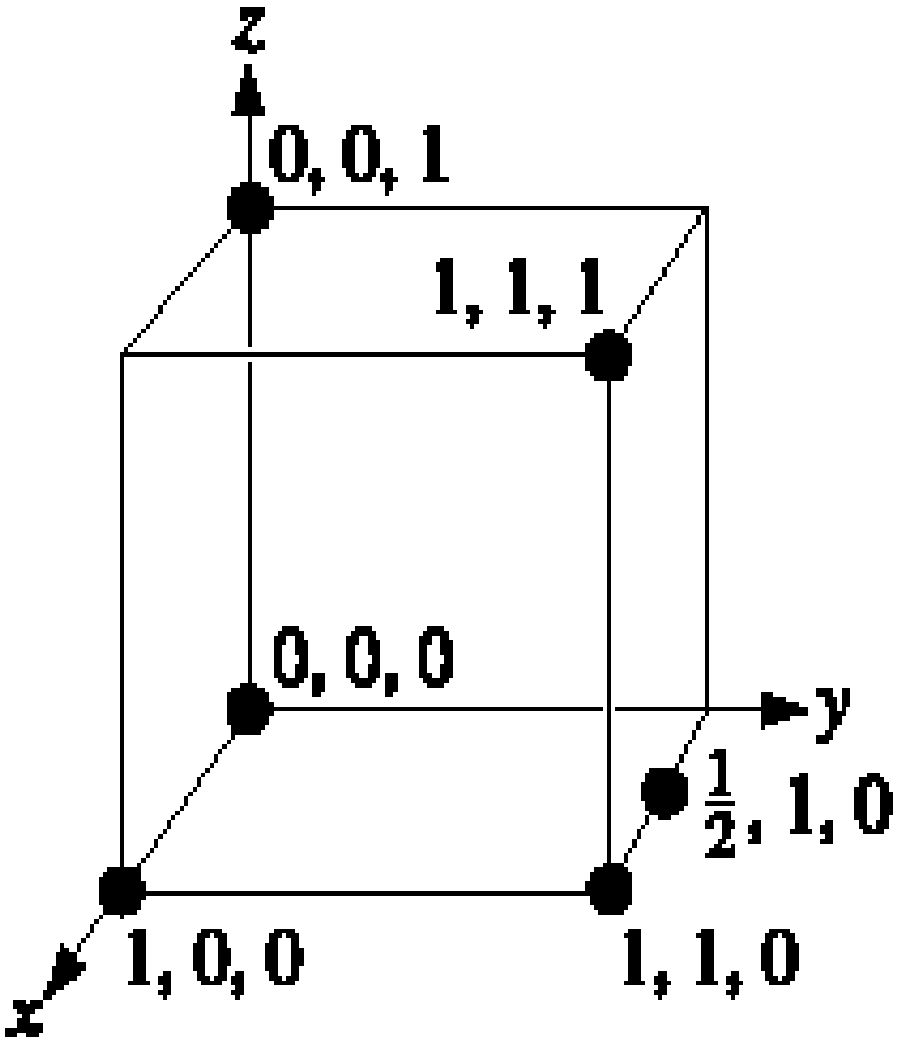
Directions of a form (also called family) - Crystallographic directions that all have the same characteristics, although their ‘‘sense’’ may be different. Denoted by < > brackets, they are symmetrically equivalent

Lattice Planes in the Unit Cell **are an altogether different matter !**

- Miller-indices - A shorthand notation to describe certain crystallographic directions and planes in a material.

Lattice planes are represented by the vector that is normal (perpendicular to them), these are 3D vectors in reciprocal (or dual) space (reciprocal space is nothing fancy - it is just a mathematical convenience !)

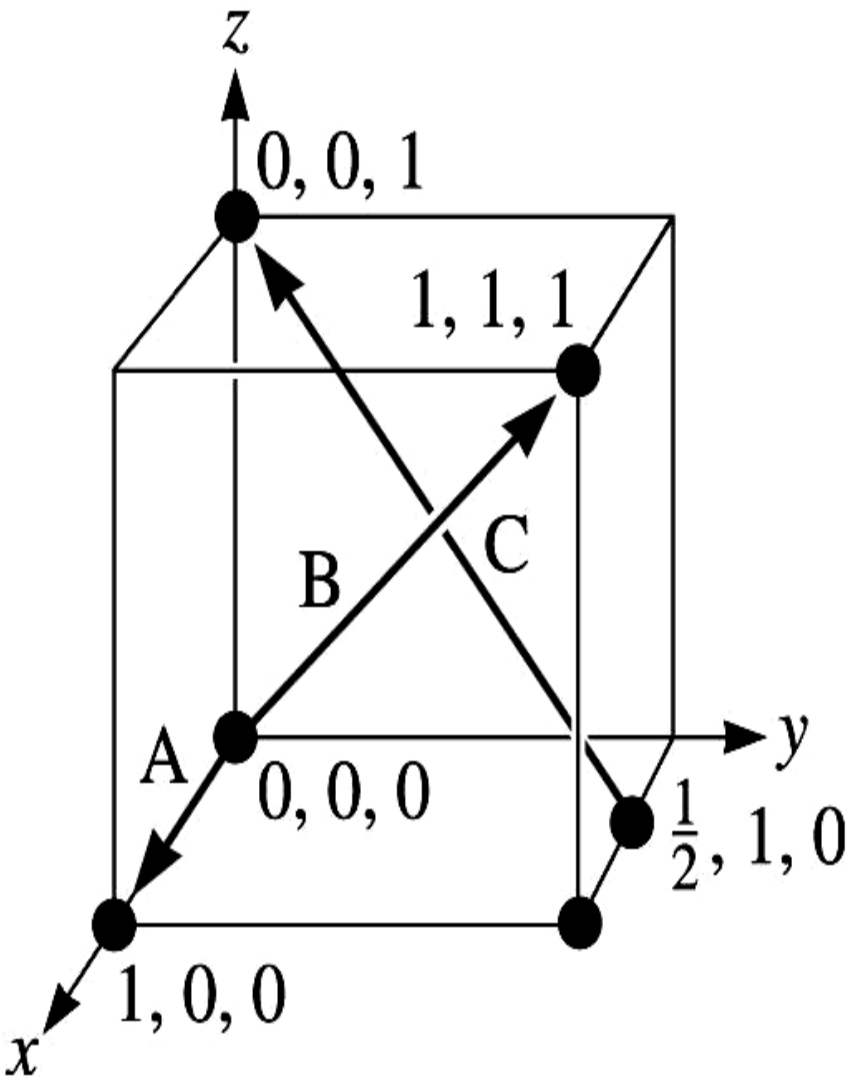
Directions of a form (also called family) – lattice planes that all have the same characteristics, although their ‘‘sense’’ may be different. Denoted by { } brackets, they are symmetrically equivalent. Now if the lattice point represents more than one point the front side and the back side of one and the same plane may have very different chemical properties as different atoms will be exposed, e.g. ZnS structure



We start with the coordinates of lattice points in order to define the Miller indices of lattice directions

Coordinates of selected points in the unit cell. The number refers to the distance from the origin in terms of lattice parameters.

Determining Miller Indices of Directions



Determine coordinates of two points that lie in direction of interest,
$u_1\ v_1\ w_1$ and $u_2\ v_2\ w_2$

calculations are simplified if the second point corresponds with the origin of the coordinate system

Subtract coordinates of second point from those of first point
$u' = u_1-u_2$, $v' = v_1-v_2$, $w' = w_1-w_2$

Clear fractions from the differences to give indices in lowest integer values. Write indices in [] brackets. Negative integer values are indicated with a bar over the integer,

[uvw] and $[\bar{u}\bar{v}\bar{w}]$ are running in opposite directions

Direction *A*

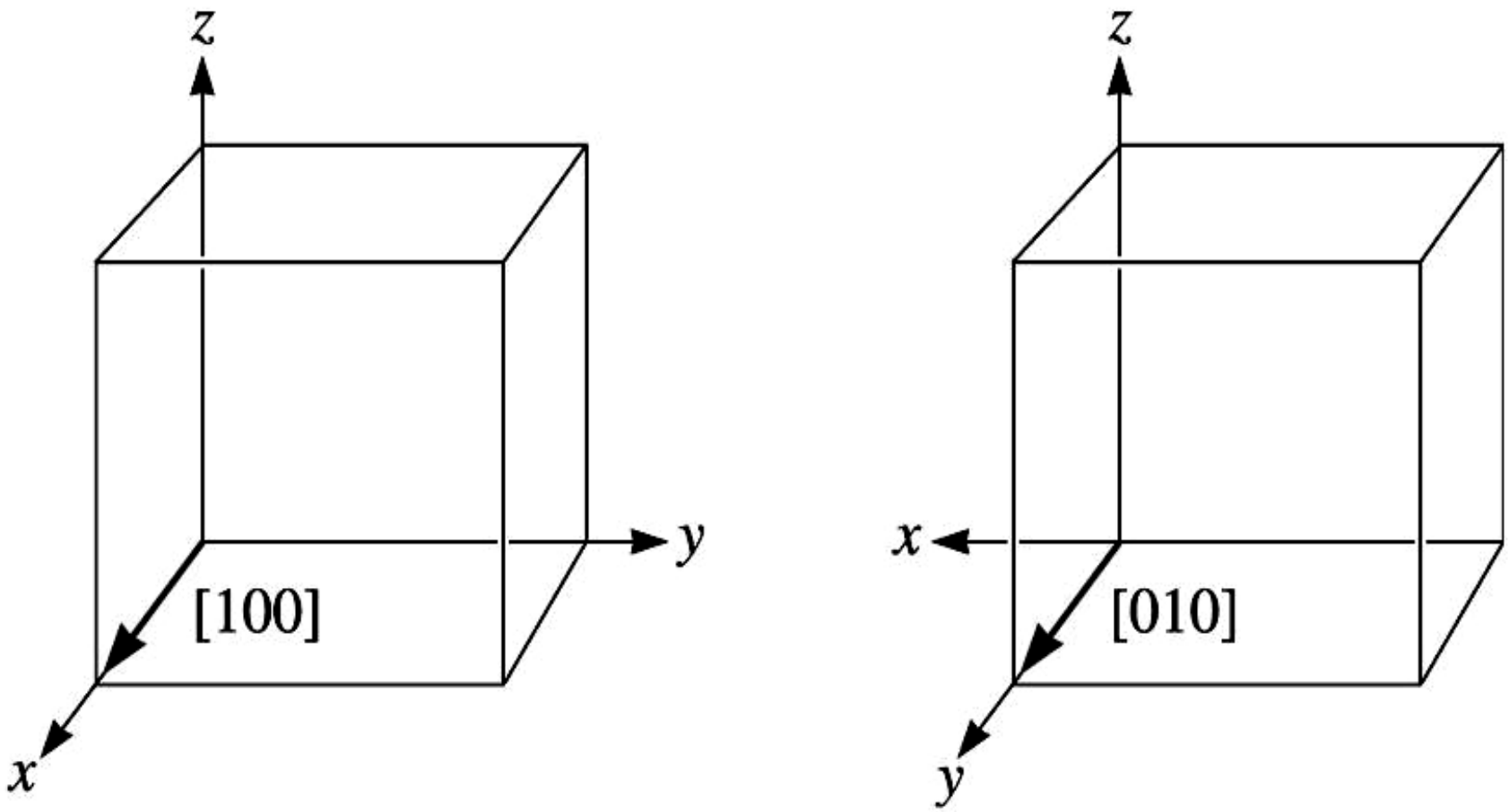
1. Two points are 1, 0, 0, and 0, 0, 0
2. 1, 0, 0, - (0, 0, 0) = 1, 0, 0
3. No fractions to clear or integers to reduce
4. [100]

Direction *B*

1. Two points are 1, 1, 1 and 0, 0, 0
2. 1, 1, 1, - (0, 0, 0) = 1, 1, 1
3. No fractions to clear or integers to reduce
4. [111]

Direction *C*

1. Two points are 0, 0, 1 and 1/2, 1, 0
2. 0, 0, 1 –(1/2, 1, 0) = -1/2, -1, 1
3. 2 (-1/2, -1, 1) = -1,-2, 2
4. $[\bar{1}\bar{2}2]$

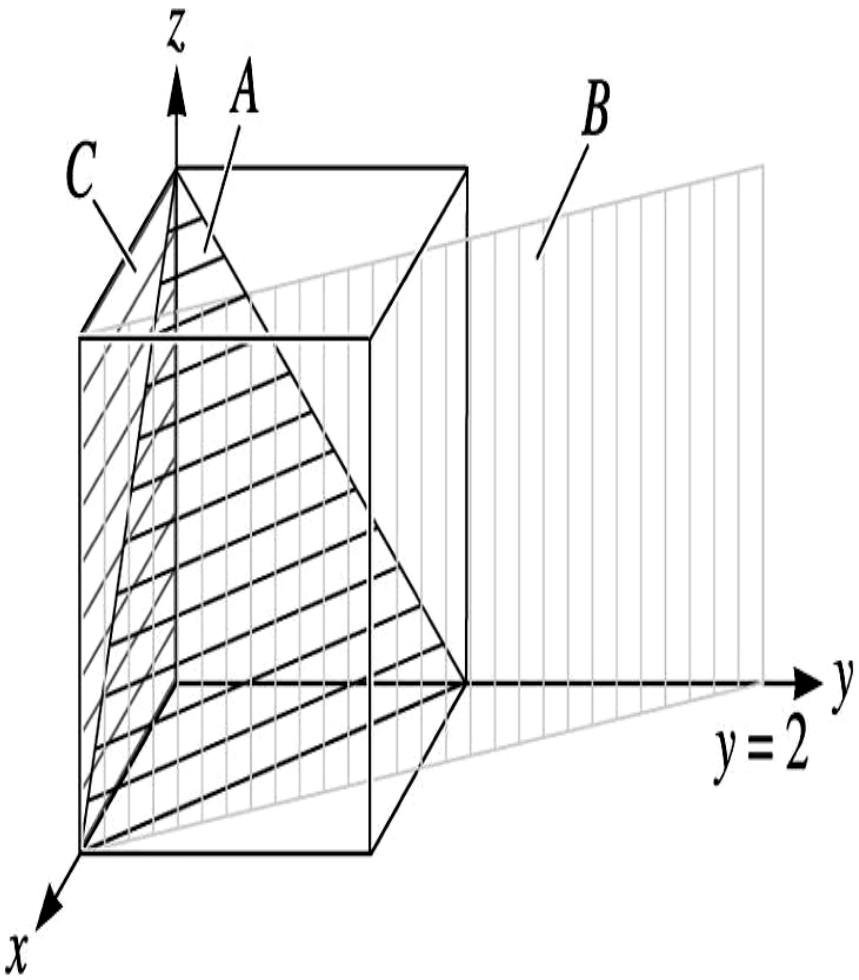


Equivalency of crystallographic directions of a form in cubic systems.

TABLE 3-3 ■ *Directions of the form* ⟨110⟩ *in cubic systems*

$$\langle 110 \rangle = \begin{cases} [110] & [\bar{1}\bar{1}0] \\ [101] & [\bar{1}0\bar{1}] \\ [011] & [0\bar{1}\bar{1}] \\ [1\bar{1}0] & [\bar{1}10] \\ [10\bar{1}] & [\bar{1}01] \\ [01\bar{1}] & [0\bar{1}1] \end{cases}$$

Determining Miller Indices of Planes



Identify the coordinate intersects of the plane, if plane is parallel to one of the axes, this intercept is taken to be infinite

Take the reciprocal of the intercept

Clear fractions, but do not reduce to lowest integers

Cite in (h k l) parentheses

Negative integer values are indicated with a bar over the integer

$(\bar{h}\ \bar{k}\ \bar{l})$ is the same plane as (h k l) , just its back side

Plane *A*

1. $x = 1$, $y = 1$, $z = 1$
2. $1/x = 1$, $1/y = 1$, $1/z = 1$
3. No fractions to clear
4. **(111)**

Plane *B*

1. The plane never intercepts the z axis, so $x = 1$, $y = 2$, and $z = \infty$
2. $1/x = 1$, $1/y = 1/2$, $1/z = 0$
3. Clear fractions: $1/x = 2$, $1/y = 1$, $1/z = 0$
4. **(210)**

Plane *C*

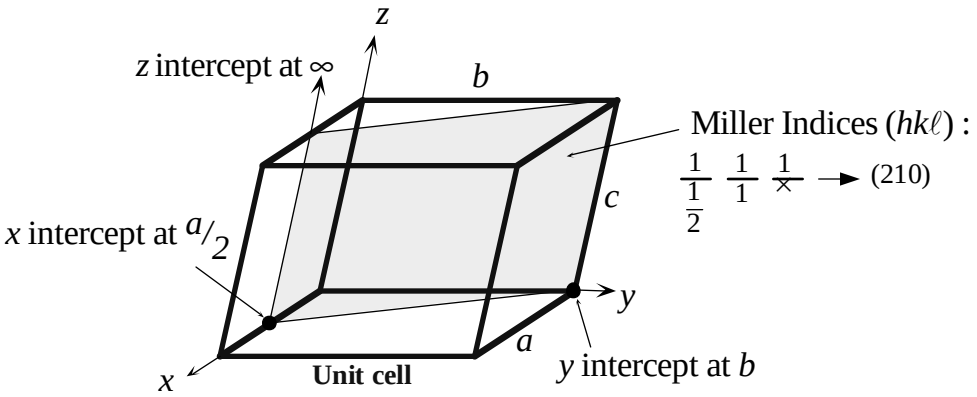
1. We shall move the origin, since the plane passes through 0, 0, 0. Let's move the origin one lattice parameter in the y-direction. Then,

$x = \infty$, $y = -1$, and $z = \infty$

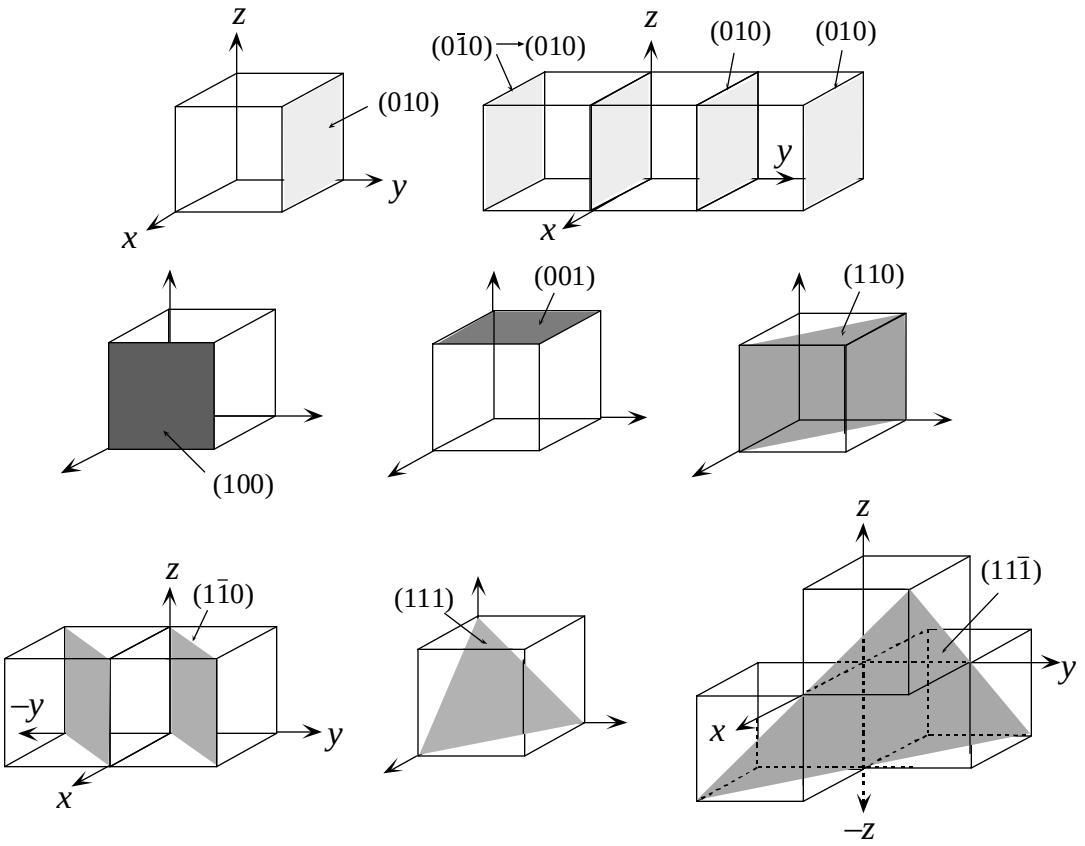
2. $1/x = 0$, $-1/y = -1$, $1/z = 0$
3. No fractions to clear.

4. $(0\bar{1}0)$

that seemed a bit arbitrary, we could have moved the origin in the –y direction as well, then we would have gotten (010), which is just the back side of $(0\bar{1}0)$



(a) Identification of a plane in a crystal



(b) Various planes in the cubic lattice

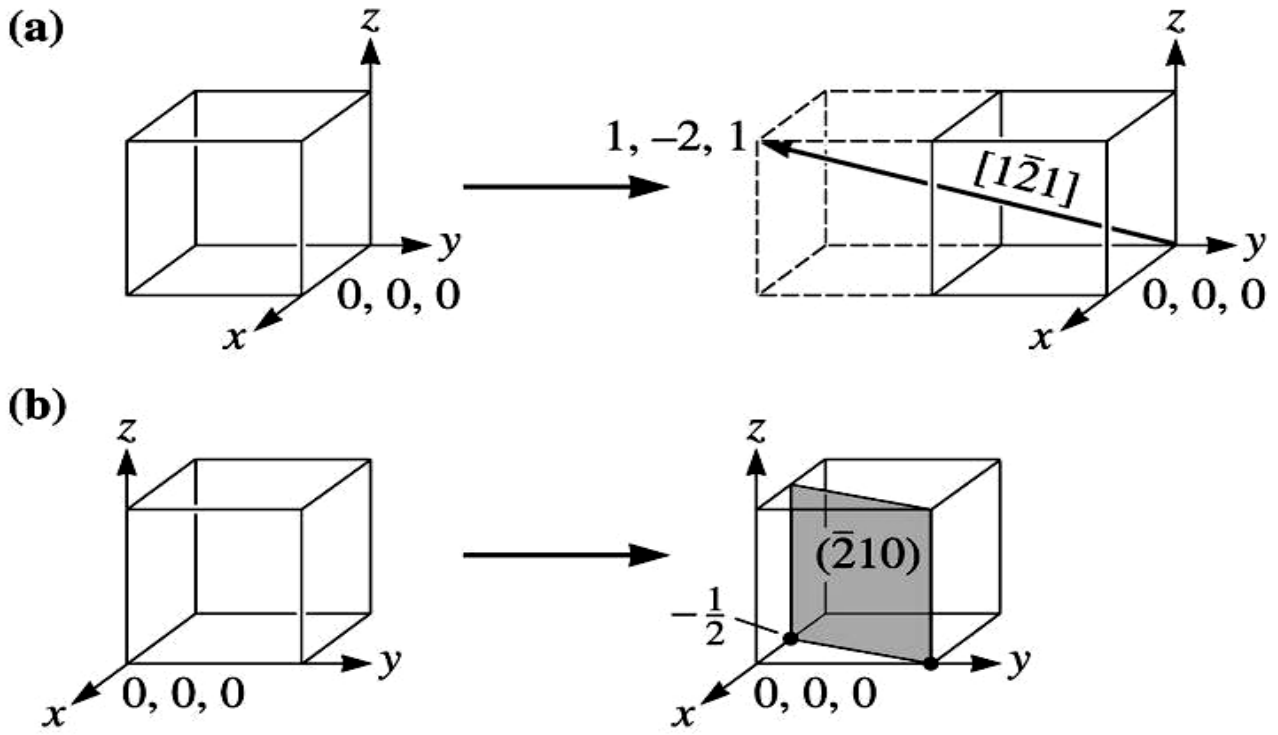
TABLE 3-4 ■ *Planes of the form {110} in cubic systems*

$$\{110\}\begin{cases}(110)\\(101)\\(011)\\(1\bar{1}0)\\(10\bar{1})\\(01\bar{1})\end{cases}$$

Note: The negatives of the planes are not unique planes.

Drawing Direction and Plane

Draw (a) the $[1\bar{2}1]$ direction and (b) the $[\bar{2}10]$ plane in a cubic unit cell.



Construction of a (a) direction and (b) plane within a unit cell

SOLUTION

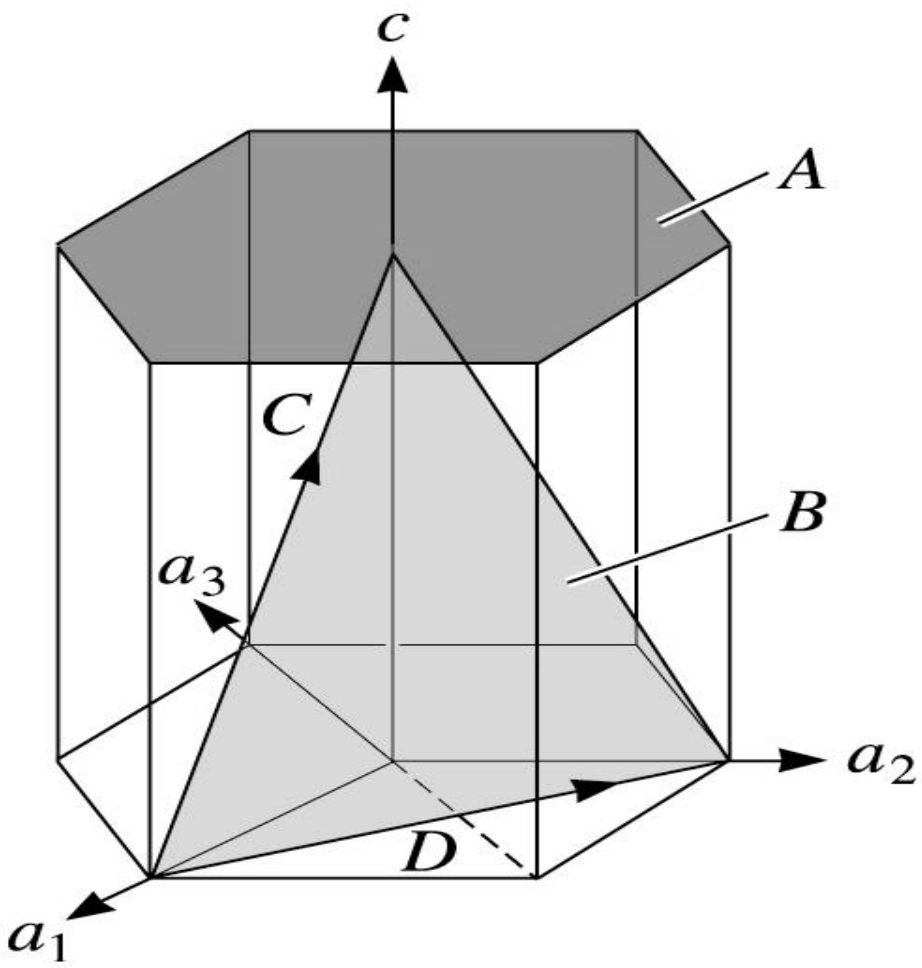
a. Because we know that we will need to move in the negative *y*-direction, let's locate the origin at 0, +1, 0. The ''tail'' of the direction will be located at this new origin. A second point on the direction can be determined by moving +1 in the *x*-direction, 2 in the negative y-direction, and +1 in the z direction.

b. To draw in the $[\bar{2}10]$ plane, first take reciprocals of the indices to obtain the intercepts, that is:

$$x = 1/-2 = -1/2 \quad y = 1/1 = 1 \quad z = 1/0 = \infty$$

Since the *x*-intercept is in a negative direction, and we wish to draw the plane within the unit cell, let's move the origin +1 in the *x*-direction to 1, 0, 0. Then we can locate the *x*-intercept at 1/2 and the *y*-intercept at +1. The plane will be parallel to the *z*-axis.

Determining Miller-Bravais Indices for Planes and Directions in hexagonal system



Miller-Bravais indices are obtained for crystallographic planes, directions, and points in hexagonal unit cells by using a **four-axis coordinate system**.

For planes (hk*i*l), the index $i = -(h+k)$, i.e. $h+k = -i$

For directions [uv*t*w], we have also $t = (u+v)$, i.e. $u+v = -t$

Miller-Bravais indices for planes are straightforward, just as we obtained the intersects for 3 axes, we have to obtain them now for 4 axes

SOLUTION

Plane *A*

1. $a_1 = a_2 = a_3 = \infty$, $c = 1$
2. $1/a_1 = 1/a_2 = 1/a_3 = 0$, $1/c = 1$
3. No fractions to clear
4. (0001)

Plane *B*

1. $a_1 = 1$, $a_2 = 1$, $a_3 = -1/2$, $c = 1$
2. $1/a_1 = 1$, $1/a_2 = 1$, $1/a_3 = -2$, $1/c = 1$
3. No fractions to clear
4. $(11\bar{2}1)$

***Determining directions in the hexagonal system is a bit more challenging* it is easier to calculate with 3 indices and then simply make up the forth**

SOLUTION (Continued)

Direction *C*

1. Two points are 0, 0, 1 and 1, 0, 0.
2. 0, 0, 1, - (1, 0, 0) = -1, 0, 1
3. No fractions to clear or integers to reduce.
4. $[\bar{1}01]\text{or}[\bar{2}113]$

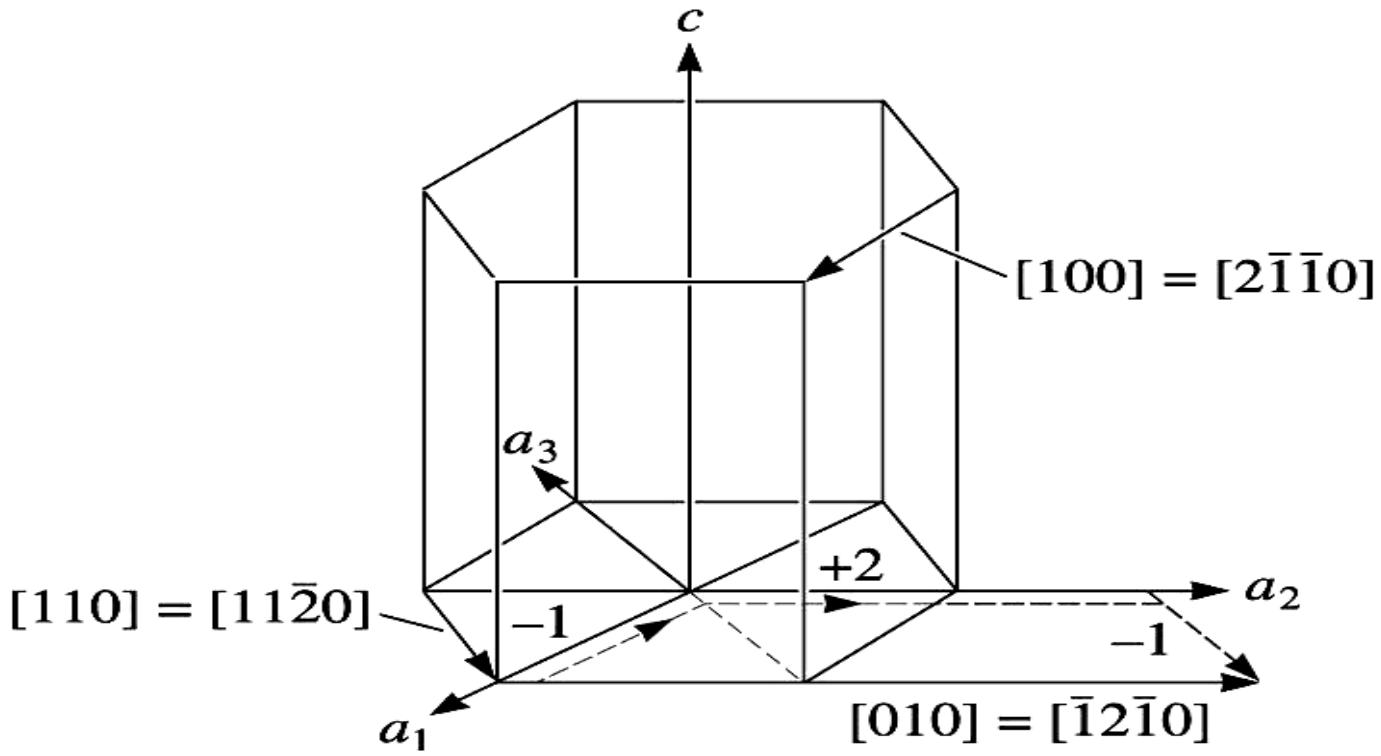
Direction *D*

1. Two points are 0, 1, 0 and 1, 0, 0.
2. 0, 1, 0, - (1, 0, 0) = -1, 1, 0
3. No fractions to clear or integers to reduce.
4. $[\bar{1}10]\text{or}[\bar{1}100]$ extension to 4 indices looks easy, but is not !

How did we get the forth index ? All have to be relabeled, say [UVW] are the three indexes, u = $^1/_3$ (2U –V),

v = $^1/_3$ (2V-U), t = - $^1/_3$ (u+v), w = W

Miller-Bravais Indices of important directions



Typical directions in the hexagonal unit cell, using both three-and-four-axis systems. The dashed lines show that the [$\bar{1}$2$\bar{1}$0] direction is equivalent to a [010] direction.

Densely packed lattice directions in the basal plane (0001), e.g. [100], [010], and [110] have similar Miller-Bravais indices, important for dislocation slip systems