

# 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.

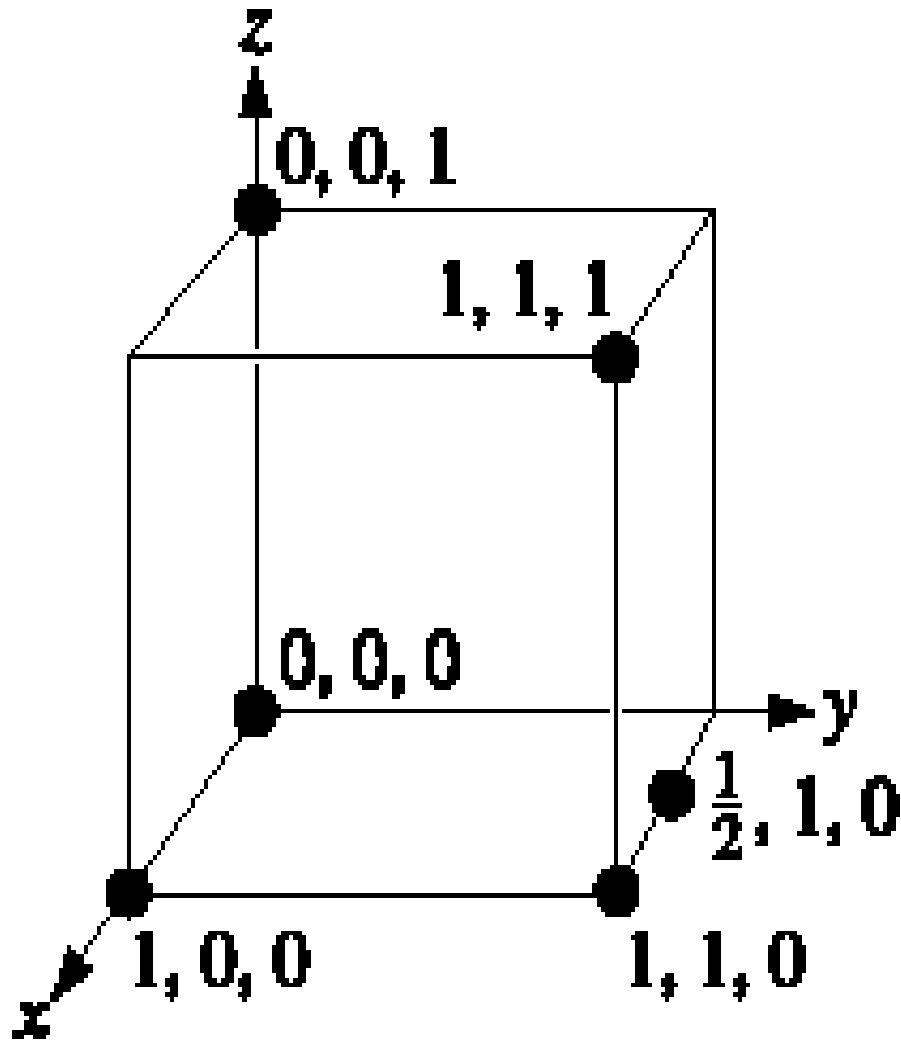
Directions of a form (also called family) - Crystallographic directions that all have the same characteristics, although their "sense" may be different. Denoted by < > brackets, they are symmetrically equivalent

# 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 !)

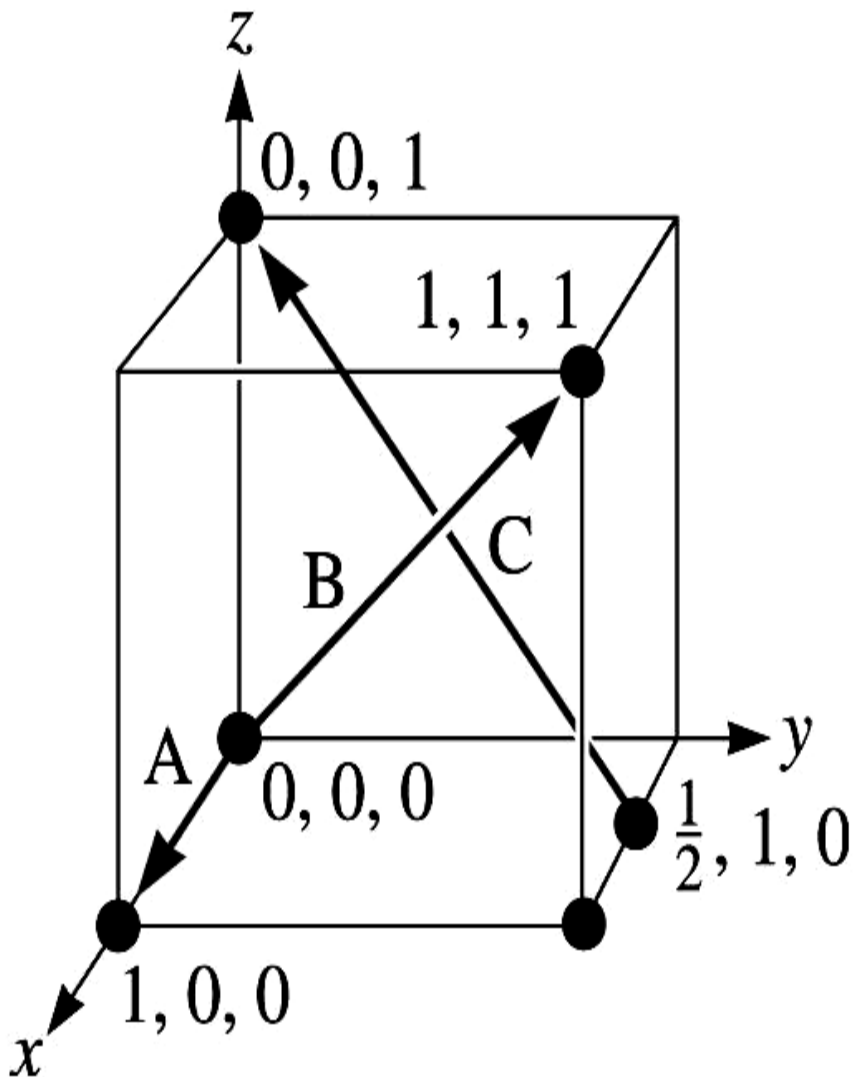
Directions of a form (also called family) – lattice planes that all have the same characteristics, although their “sense” may be different. Denoted by  $\{ \}$  brackets, they are symmetrically equivalent. Now if the lattice point represents more than one point the front side and the back side of one 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

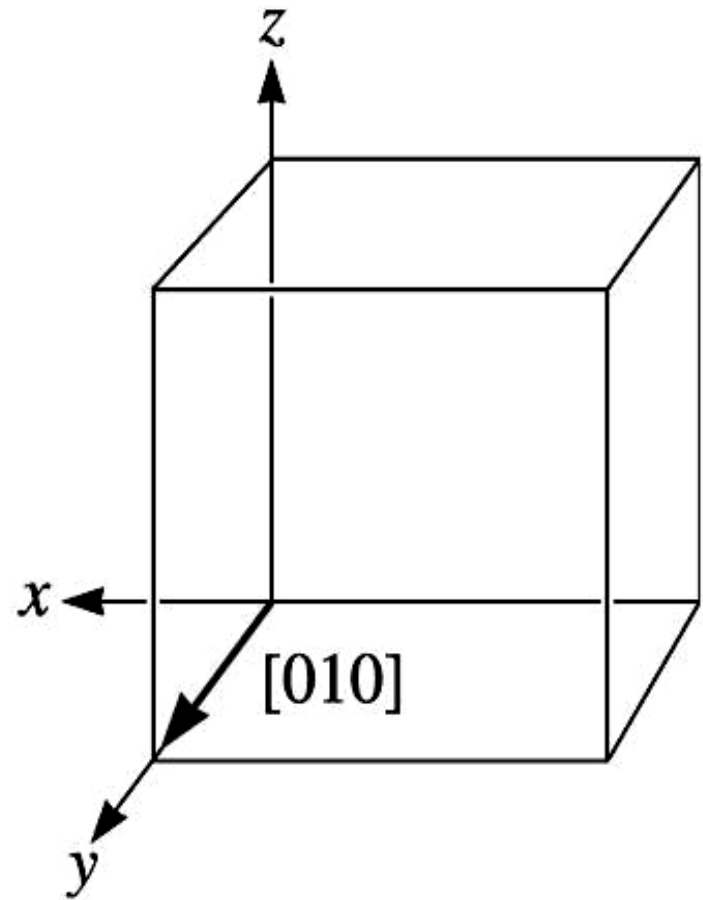
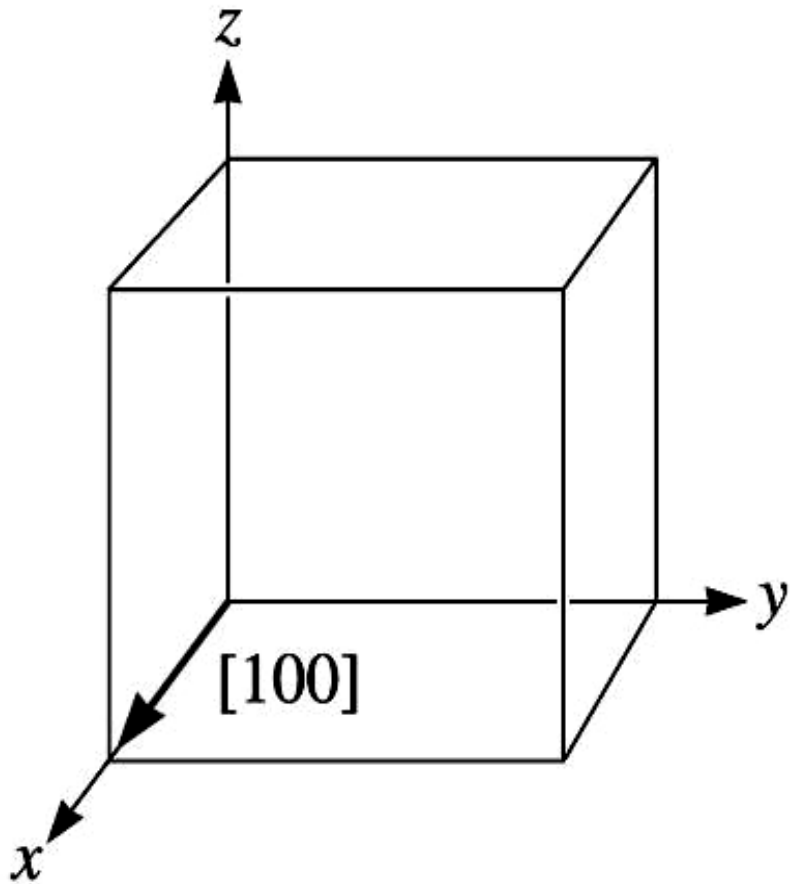
1. Two points are 1, 0, 0, and 0, 0, 0
2.  $1, 0, 0, - (0, 0, 0) = 1, 0, 0$
3. No fractions to clear or integers to reduce
4. [100]

## 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.

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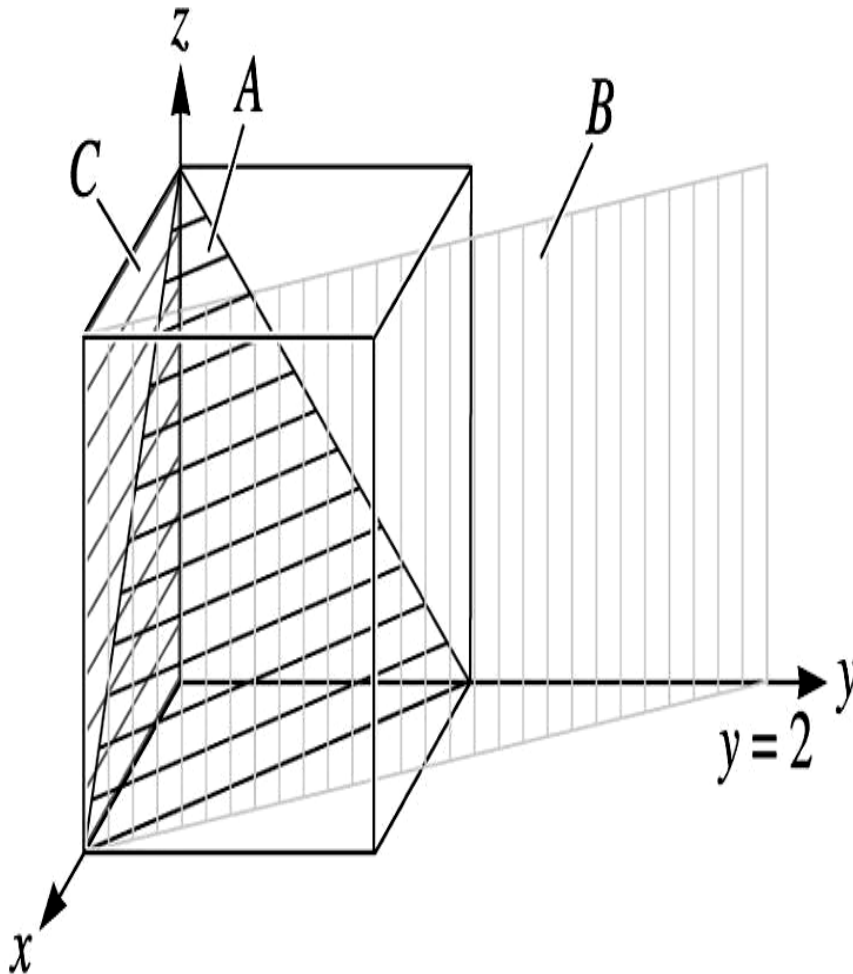
**TABLE 3-3 ■ Directions of the form  $\langle 110 \rangle$  in cubic systems**

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$$\langle 110 \rangle = \left\{ \begin{array}{ll} [110] & [\bar{1}\bar{1}0] \\ [101] & [\bar{1}0\bar{1}] \\ [011] & [0\bar{1}\bar{1}] \\ [1\bar{1}0] & [\bar{1}10] \\ [10\bar{1}] & [\bar{1}01] \\ [01\bar{1}] & [0\bar{1}1] \end{array} \right.$$

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# Determining Miller Indices of Planes



Identify the coordinate intercepts 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)**

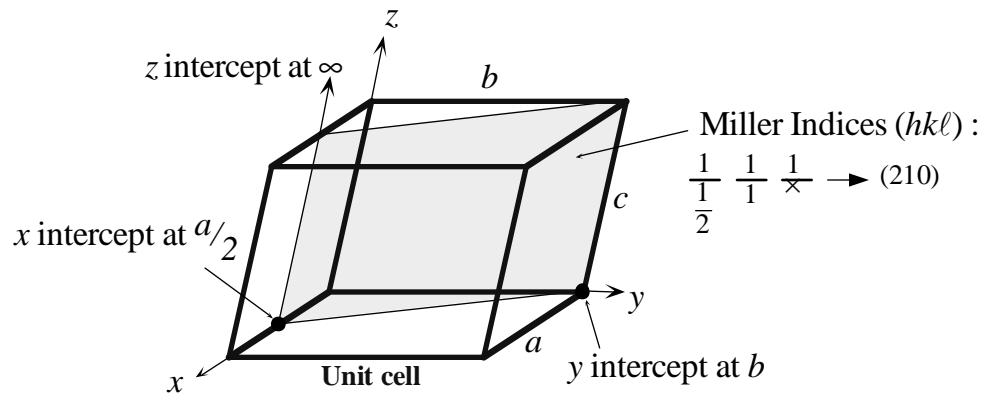
## Plane B

1. The plane never intercepts the z axis, so  $x = 1, y = 2, \text{ and } z = \infty$
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)**

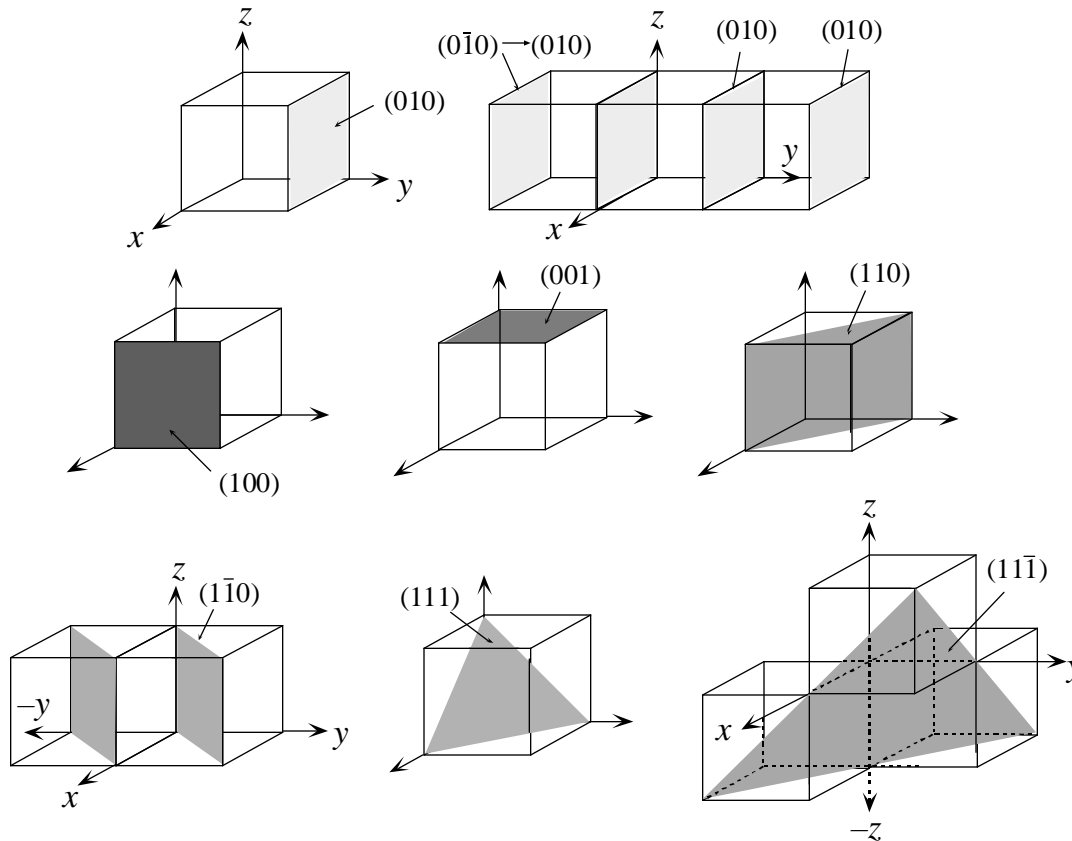
## Plane C

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,  $x = \infty, y = -1, \text{ and } z = \infty$
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

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**TABLE 3-4 ■ Planes of the form {1 1 0} in cubic systems**

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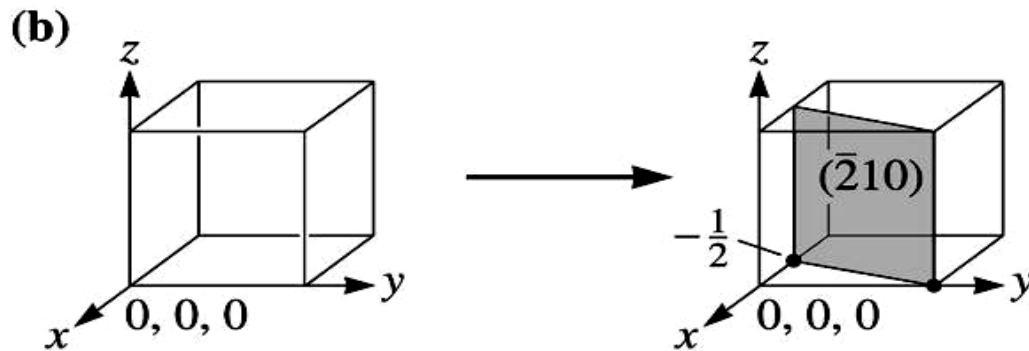
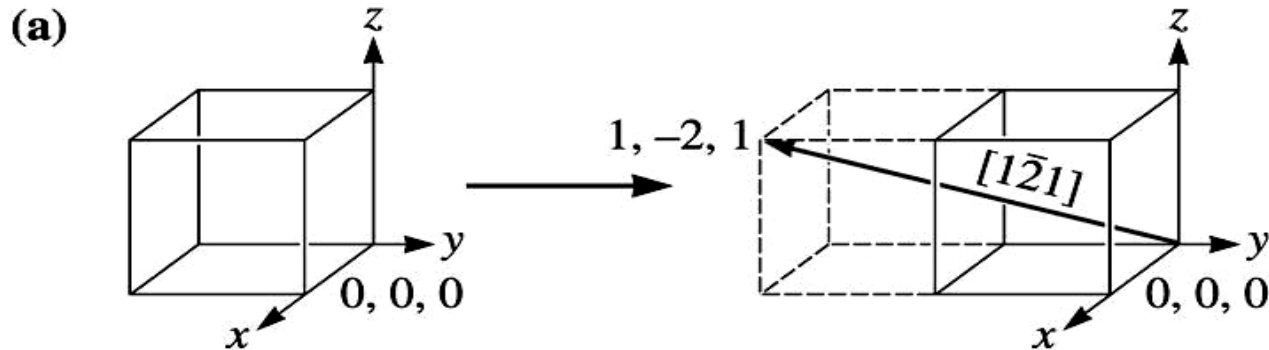
$$\{110\} \left\{ \begin{array}{l} (110) \\ (101) \\ (011) \\ (1\bar{1}0) \\ (10\bar{1}) \\ (01\bar{1}) \end{array} \right.$$

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

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# 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.

**Same basic idea for lattice planes, i.e. their normals which are vectors in reciprocal (or dual) space**  
**everything is easy in cubic systems, in other crystal systems we use reciprocal metric tensor, the reciprocal 3 by 3 matrix of the metric tensor**

$$\begin{pmatrix} b^2c^2 \sin^2 a & abc^2(\cos a \cos b - \cos g) & ab^2c(\cos a \cos g - \cos b) \\ abc^2(\cos a \cos b - \cos g) & a^2c^2 \sin^2 b & a^2bc(\cos b \cos g - \cos a) \\ ab^2c(\cos a \cos g - \cos b) & a^2bc(\cos b \cos g - \cos a) & a^2b^2 \sin^2 g \end{pmatrix}$$

**If cubic simply, this also defines the reciprocal lattice**

$$\begin{pmatrix} 1/a^2 & 0 & 0 \\ 0 & 1/a^2 & 0 \\ 0 & 0 & 1/a^2 \end{pmatrix}$$

**So angle between normals of lattice planes become**

$$\mathbf{a} = \arccos \frac{h'Gk}{\sqrt{h'Gh} \sqrt{k'Gk}}$$

## Metric tensor (and its reciprocal) also define reciprocal lattice

$$a^* = (\sqrt{b^2 c^2 \sin^2 \mathbf{a}})^{-1} = b \times c$$

$$b^* = (\sqrt{a^2 c^2 \sin^2 \mathbf{b}})^{-1} = a \times c$$

$$c^* = (\sqrt{b^2 a^2 \sin^2 \mathbf{g}})^{-1} = b \times a$$

It is just a mathematical convenience, particularly useful for interpretation of (X-ray and electron diffraction) data

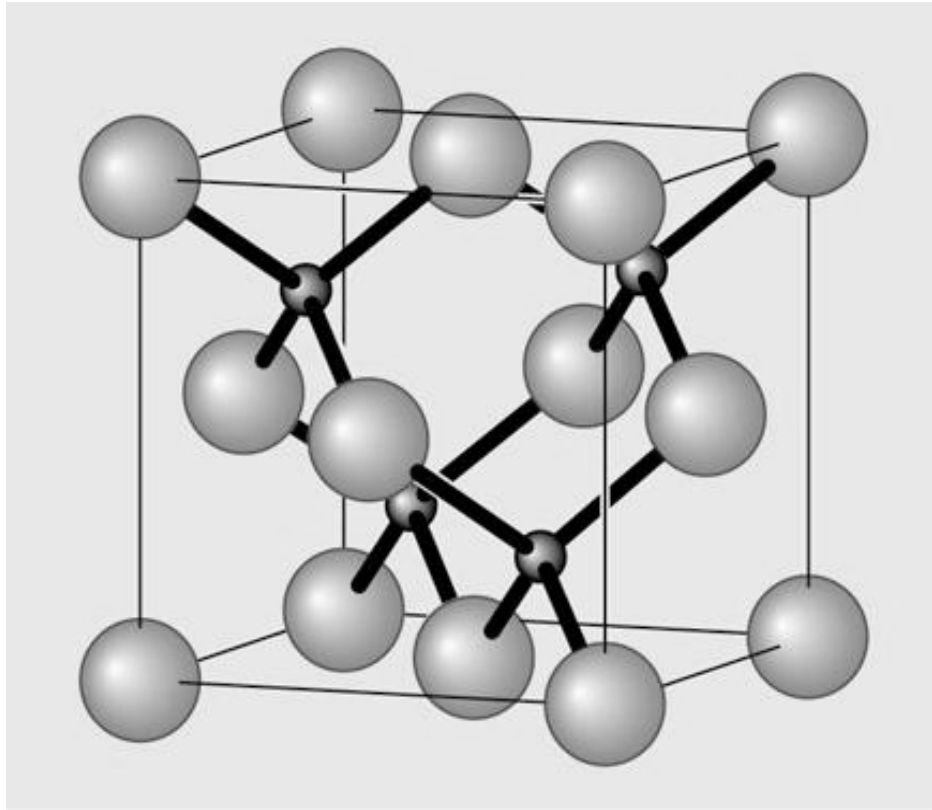
$$d^* = H = h a_1^* + k a_2^* + l a_3^* = 1/d$$

In cubic systems simply: 
$$d_{hkl} = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$$

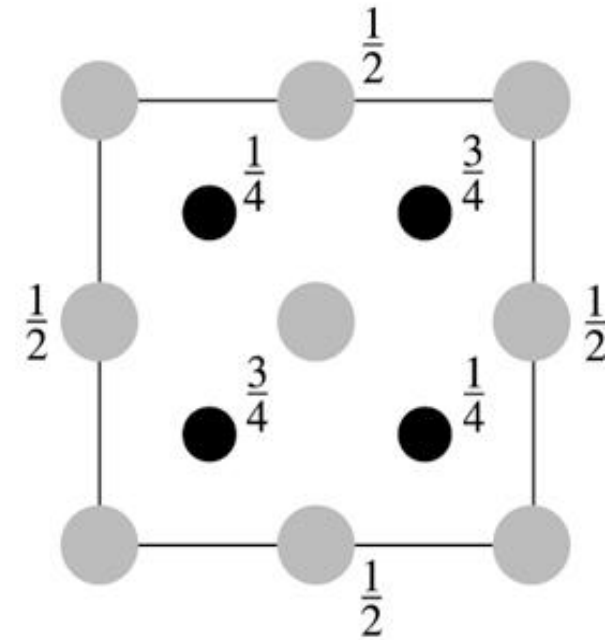
# Covalent Structures

- Covalently bonded materials frequently have complex structures in order to satisfy the directional restraints imposed by the bonding.
- Diamond cubic (DC) - A special type of face-centered cubic crystal structure found in carbon, silicon,  $\alpha$ -Sn, and other covalently bonded materials.





(a)



(b)

(a) The zinc blende unit cell, (b) plan view. There is usually a large covalent contribution to these bonds. The coordination is quite low for ionic bonds.

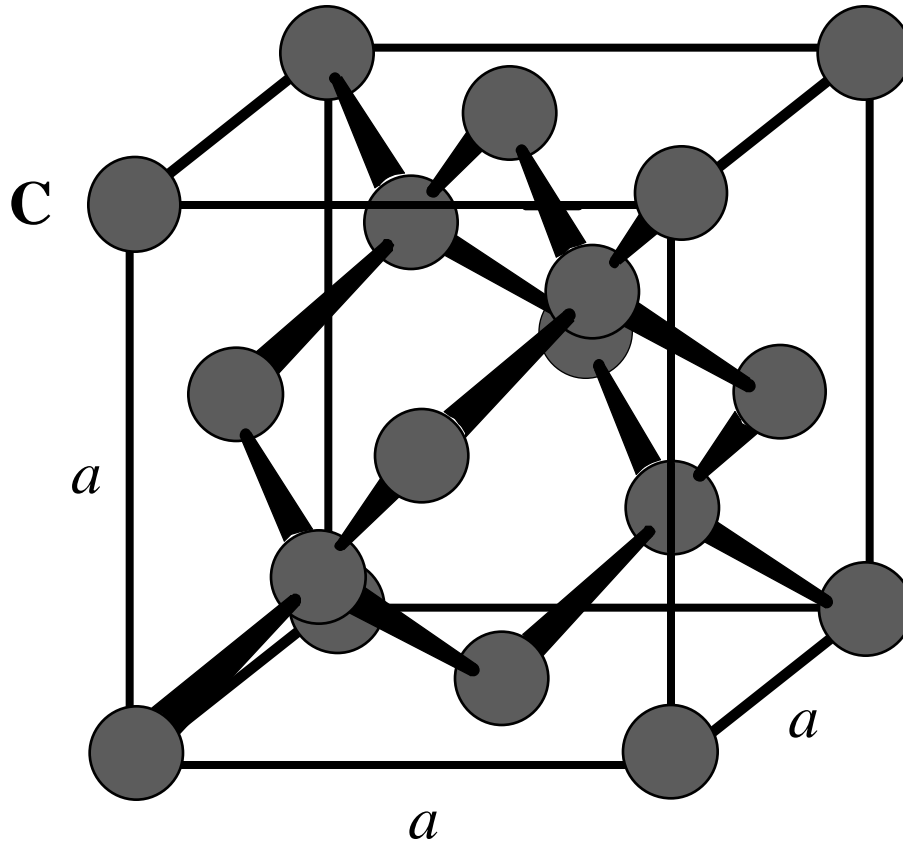


Fig. 1.33: The diamond unit cell is cubic. The cell has eight atoms. Grey Sn ( $\alpha$ -Sn) and the elemental semiconductors Ge and Si have this crystal structure.

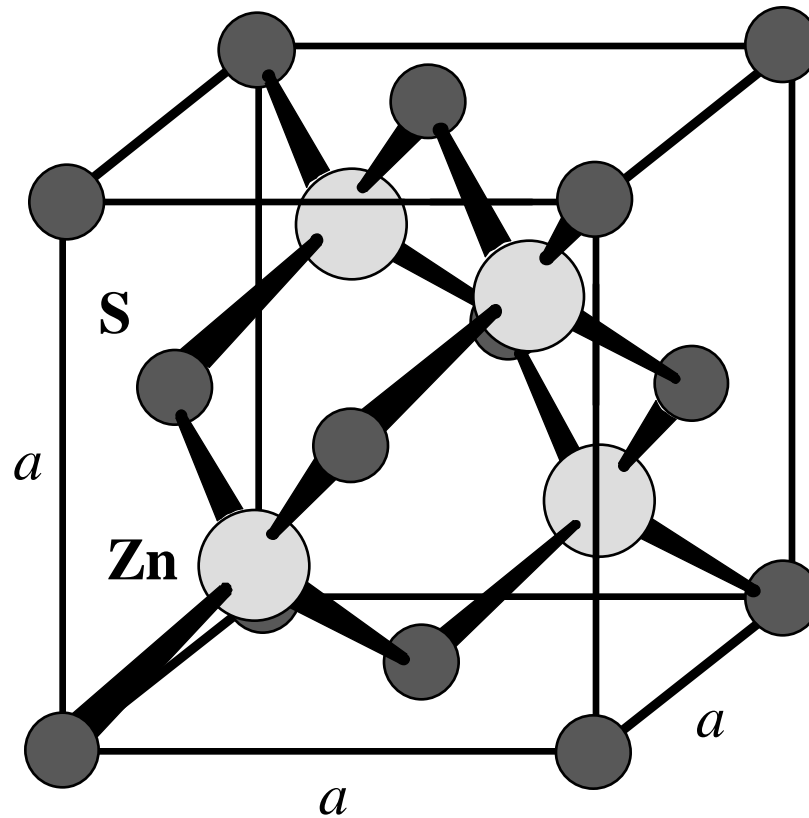


Fig. 1.34: The Zinc blende (ZnS) cubic crystal structure. Many important compound crystals have the zinc blende structure. Examples: AlAs, GaAs, GaP, GaSb, InAs, InP, InSb, ZnS, ZnTe.